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INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

LINTAB, HEATER and PLOTTAB code package

Computer codes for model parameters and cross-section data.

(version 87-1)

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This document describes a series of computer codes for computing cross-section data from model parameters.

Abstract: The code LINTAB produces linearly interpolable tables of cross-sections from nuclear or atomic models. - The code HEATER calculates spectrum averaged reaction rates from linearly interpolable cross-section tables. - The code PLOTTAB plots and compares various data tables.

These codes were prepared as a support package for atomic and molecular data, but they are also applicable to nuclear and other data.

Upon request, the programs are available costfree from the IAEA Nuclear Data Section.

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B = 3.865, -4.605, 1.543

LINTAB, HEATER and PLOTTAB code package

(version 87-1)

Introduction

At the present time this package is composed of three computer programs. These programs are being continuously extended to include additional cross section and weighting spectrum models.

1) LINTAB - Starting from a model construct linearly interpolable tables of cross sections.

2) HEATER - Starting from linearly interpolable tables of cross sections (i.e., LINTAB output) calculate spectrum averaged reaction rates in linearly interpolable tabular form.

3) PLOTTAB - Starting from linearly interpolable tables (i.e., LINTAB or HEATER output) and/or experimentally measured point values produce plots comparing up to 30 sets of tables and/or sets of point values.

Documentation

The programs in this package are designed to be self documenting, in the sense that all details of the methods, input/output, etc. used by each programs are described on comment cards at the beginning of each program.

This document contains a copy of the comment cards from each program as of July, 1987. The user should be aware that the comment cards in the programs are continuously updated and at any given time are the most up to date documentation for the codes and may supersede published documentation (such as this report). Therefore before implementing and using these programs the user should read the comment cards at the beginning of the program.

Program LINTAB

PROGRAM LINTAB(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10)

PROGRAM LINTAB
VERSION 87-1 (JULY, 1987)

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PURPOSE
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CONSTRUCT LINEARLY INTERPOLABLE TABLE FROM ANY FUNCTION.

INTRODUCTION

THIS PROGRAM WILL START FROM ANY FUNCTION OF A SINGLE CONTINUOUS VARIABLE...FUNKY(X). BY USER INPUT THE FUNCTION CAN BE DEFINED,

(1) OVER 1 TO 100 X RANGES,
(2) WITHIN EACH X RANGE THE FUNCTION IS DEFINED BY 0 TO 50 CONSTANTS.
(3) AT BOUNDARIES BETWEEN X RANGES THE FUNCTION MAY BE CONTINUOUS OR DISCONTINUOUS (DEPENDING ON THE CONSTANTS USED TO DEFINE THE FUNCTION WITHIN EACH X RANGE).

THE PROGRAM WILL CONSTRUCT A TABLE OF X AND Y VALUES WHERE THE TABULATED (X,Y) PAIRS WILL BE EXACTLY EQUAL TO THE FUNCTION (E.G., Y=FUNKY(X)) AND LINEAR INTERPOLATION BETWEEN THE TABULATED PAIRS WILL BE WITHIN ANY USER SPECIFIED FRACTIONAL UNCERTAINTY OF THE FUNCTION FOR ALL VALUES OF X WITHIN THE REQUESTED X RANGE.
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WHY

FOR MANY APPLICATIONS IT IS MORE CONVENIENT TO WORK WITH A TABLE (OR TABLES) DEFINING A FUNCTION THAN WITH THE ACTUAL FUNCTION. FOR EXAMPLE,

(1) WHEN THE FUNCTION IS COMPLICATED AND IS USED MANY TIMES IN APPLICATIONS IT MAY BE FASTER AND CHEAPER TO FIRST CONSTRUCT A TABLE AND THEN PERFORM TABLE LOOKUP DURING APPLICATION.
(2) WHEN THE FUNCTION IS COMPLICATED AND ITS INTEGRAL IS REQUIRED, EVEN IF THE FUNCTION CAN BE ANALYTICALLY INTEGRATED IT IS OFTEN CHEAPER AND MORE ACCURATE (DUE TO POSSIBLE NUMERICAL INSTABILITIES IN THE DEFINITION OF THE ANALYTICAL INTEGRAL) TO START FROM A LINEARLY INTERPOLABLE TABLE TO DEFINE THE INTEGRAL IN A COMPLETELY NUMERICALLY STABLE FORM. WHEN THE INTEGRAL OF A FUNCTION CANNOT BE DEFINED IN ANALTYICAL FORM TABULATING THE FUNCTION AND INTEGRATING THE TABULATED RESULTS MAY BE THE ONLY PRACTICAL APPROACH.
(3) TO COMPARE A NUMBER OF DIFFERENT MODELS AND IN PARTICULAR TO QUANTITATIVELY DEFINE THE DIFFERENCES BETWEEN THE RESULTS OBTAINED USING EACH MODEL IT IS CONVENIENT TO TABULATE THE RESULTS OBTAINED USING EACH MODEL AND TO THEN PERFORM A SIMPLE COMPARISON OF THE TABULATED RESULTS (E.G., SEE PROGRAM PLOTTAB...WHICH IS DESIGNED TO PERFORM SUCH COMPARISONS).

ALLOWABLE UNCERTAINTY

IN GENERAL A FUNCTION CANNOT BE EXACTLY REPRESENTED IN TABULATED LINEARLY INTERPOLABLE FORM. HOWEVER, MANY FUNCTIONS CAN BE REPRESENTED IN THIS FORM TO WITHIN AN ACCURACY WHICH IS ADEQUATE TO MEET THE NEEDS OF ANY APPLICATION. IN PARTICULAR WHEN DEALING WITH PHYSICAL DATA WHICH HAS AN INHERENT UNCERTAINTY ASSOCIATED

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WITH IT, IT IS USUALLY POSSIBLE TO TABULATE RESULTS WHICH DIFFER FROM THE MODEL'S RESULTS BY CONSIDERABLY LESS THAN THE INHERENT UNCERTAINTY IN THE MODEL, E.G. IF A MODEL CAN PREDICT NUCLEAR CROSS SECTIONS AT ANY ENERGY TO WITHIN 5 PER-CENT, OBVIOUSLY TABULATING CROSS SECTIONS WHICH AGREE WITH THE RESULTS OF THE MODEL TO WITHIN 0.1 PER-CENT WILL INTRODUCE A NEGLIABLE CHANGE IN THE TOTAL UNCERTAINTY OF THE RESULTS.

BY INPUT PARAMETERS THE USER SPECIFIES AN ALLOWABLE UNCERTAINTY IN EACH X RANGE. SINCE THE ACCURACY TO WHICH THE TABULATED VALUES MUST APPROXIMATE THE FUNCTION ARE APPLICATION DEPENDENT IT IS NOT POSSIBLE TO GIVE GENERAL GUIDELINES AS TO THE MAGNITUDE OF THE ALLOWABLE UNCERTAINTY. HOWEVER, IT IS POSSIBLE TO POINT OUT THAT USUALLY THE NUMBER OF TABULATED POINTS WILL NOT RAPIDLY INCREASE AS THE ALLOWABLE UNCERTAINTY IS DECREASED. AS A RULE OF THUMB THE NUMBER OF POINTS WILL ROUGHLY INCREASE IN PROPORTION TO THE RECIPROCAL OF THE SQUARE ROOT OF THE ALLOWABLE UNCERTAINTY, E.G., IF TABULATING A FUNCTION TO 1 PER-CENT ACCURACY RESULTS IN 100 POINTS, TABULATING THE SAME FUNCTION TO 0.1 PER-CENT ACCURACY WILL RESULT IN ABOUT 300 POINTS. FOR ANY GIVEN APPLICATION THE USER CAN USE THIS GUIDELINE TO DETERMINE THE BEST ALLOWABLE UNCERTAINTY TO OBTAIN A COMPROMISE BETWEEN ACCURACY AND TABLE SIZE (WHICH WILL NORMALLY EFFECT RUNNING TIME OF APPLICATIONS).

ACCURACY OF TABULATED RESULTS

IN ORDER TO MAKE THIS APPROACH PRACTICAL IT IS IMPORTANT TO INSURE THAT THE TABLE CAN ACCURATELY REPRESENT TO WITHIN A USER SPECIFIED UNCERTAINTY THE FUNCTION NOT ONLY AT VALUES AT WHICH THE FUNCTION IS TABULATED, BUT FOR ALL VALUES OF X WITHIN THE TABULATED X RANGE
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TO WITHIN A USER SPECIFIED ACCURACY, TO MEET THE NEEDS OF ANY APPLICATION. ONLY IF THIS CAN BE DONE IS IT POSSIBLE TO SPECIFY THE UNCERTAINTY IN ANY RESULTS OBTAINED WHEN THE TABLE IS USED IN APPLICATIONS, E.G. IF YOU WISH TO CALCULATE THE INTEGRAL OF A FUNCTION OVER SOME INTERVAL BY USING THE TABULATED VALUES AND INTEGRATING BETWEEN TABULATED VALUES, IF THE TABLE IS CONSTRUCTED TO ACCURATELY REPRESENT THE FUNCTION OVER THE ENTIRE RANGE OF THE INTEGRAL TO WITHIN 0.1 PER-CENT AND THE FUNCTION DOES NOT CHANGE SIGN WITHIN THE INTERVAL THE RESULTING INTEGRAL WILL BE GUARANTEED TO BE ACCURATE TO WITHIN 0.1 PER-CENT.

X RANGES

X RANGES SPECIFIED BY USER INPUT MUST BE IN ASCENDING X ORDER. IF ANY INTERVALS ARE NOT IN ASCENDING ORDER THE PROGRAM WILL PRINT A WARNING MESSAGE AND IGNORE THE X INTERVAL.

IF THE FUNCTION IS NOT ANALYTICAL OVER THE ENTIRE X RANGE THE USER SHOULD DEFINE SEPARATE X RANGES IN EACH OF WHICH THE FUNCTION IS ANALYTICAL.

THE RUNNING TIME OF THE PROGRAM CAN BE MINIMIZED BY SPECIFYING X RANGES EACH OF WHICH DO NOT CONTAIN TOO MANY MINIMA AND MAXIMA.

EACH X RANGE SPECIFIED ON INPUT WILL BE TREATED SEPARATELY BY THE PROGRAM. FOR EACH X RANGE THE PROGRAM WILL TABULATE THE FUNCTION FOR X VALUES BETWEEN THE LOWER X LIMIT OF THE CURRENT X RANGE AND THE LOWER X LIMIT OF THE NEXT X RANGE (NOTE, FOR N X RANGES THE USER MUST INPUT N+1 X LIMITS, THE FIRST N X LIMITS SPECIFYING THE LOWER X LIMIT OF THE RANGE AND THE N+1 X LIMIT SPECIFYING THE UPPER X LIMIT OF THE LAST X RANGE). AT THE BOUNDARY BETWEEN X RANGES IF THE FUNCTION IS CONTINUOUS THE PROGRAM WILL ONLY OUTPUT THE (X,Y) ONCE. IF THE FUNCTION IS DISCONTINUOUS THE PROGRAM WILL

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39 4.17046+ 1 1.00173-16 2.16270-18-9.16067-20

OUTPUT THE SAME VALUE OF X TWICE AND THE VALUE OF THE FUNCTION IN EACH OF THE TWO X RANGES.

WITHIN EACH X RANGE THE FUNCTION MAY BE TABULATED AT UP TO 2000 X VALUES. IF THIS NUMBER IS EXCEEDED THE PROGRAM WILL PRINT AN ERROR MESSAGE AND PROCEED TO THE NEXT X RANGE. IF THIS OCCURS IN ANY X RANGE THE USER SHOULD SUB-DIVIDE THE X RANGE INTO A NUMBER OF SMALLER X RANGES AND RE-RUN THE PROGRAM (NOTE, SINCE UP TO 100 X RANGES ARE ALLOWED THIS PROGRAM CAN BE USED TO TABULATE ANY FUNCTION AT UP TO 200,000 POINTS).

X INTERVALS

WITHIN EACH X RANGE THE PROGRAM WILL DEFINE X INTERVALS FROM WHICH IT WILL START THE ITERATIVE INTERVAL HALVING ALGORITHM (DESCRIBED BELOW). THE X INTERVALS WILL BE DEFINED TO DIVIDE EACH X RANGE INTO AT LEAST 100 X INTERVALS USING ONE OF THE FOLLOWING METHODS,

(1) IF THE LOWER X LIMIT OF THE CURRENT X RANGE IS NOT POSITIVE, OR THE UPPER X LIMIT OF THE RANGE IS LESS THAN 10 TIMES THE LOWER X LIMIT THE X INTERVALS WILL BE LINEAR IN X (E.G., AN INTERVAL WILL BE 1/100 THE UPPER MINUS THE LOWER X LIMIT). NOTE, BY SPECIFYING MORE, SMALLER X RANGES THE USER CAN FORCE THE PROGRAM TO USE THIS OPTION).

(2) OTHERWISE THE X INTERVALS WILL BE LOGARITMICALLY SPACED IN X (E.G. AN INTERVAL WILL BE 1/100 OF THE LOG OF THE UPPER OVER THE LOWER X LIMIT). NOTE, FOR X RANGES WHICH EXTEND OVER MANY ORDERS OF MAGNITUDE (E.G., ENERGY FROM 1 EV TO 500 KEV) THIS OPTION WILL GIVEN EQUAL IMPORTANCE TO EACH DECADE OF X.

THE 100 X INTERVALS IN EACH X RANGE ARE DESIGNED TO GIVE A GOOD INITIAL APPROXIMATION TO THE SHAPE OF THE FUNCTION. IN ORDER TO INSURE THAT THE METHOD PROPERLY CONVERGES AND FINDS ALL MAXIMA AND MINIMA OF THE FUNCTION THE USER SHOULD DEFINE X RANGES SUCH THAT THERE IS NOT MORE THAN 1 MAXIMUM OR MINIMUM IN EACH X INTERVAL (NOTE, 1 PER X INTERVAL WHICH ALLOWS UP TO 100 PER X RANG).

INTERVAL HALVING

IN ORDER TO CONSTRUCT A LINEARLY INTERPOLABLE TABLE THIS PROGRAM WILL CALCULATE THE FUNCTION AT THE ENDS OF AN X INTERVAL AND AT THE MIDPOINT OF THE X INTERVAL IT WILL CALCULATE THE FUNCTION AND THE VALUE OBTAINED BY LINEARLY INTERPOLATING BETWEEN THE VALUES OF THE FUNCTION AT THE ENDS OF THE INTERVAL. IF AT THE MIDPOINT OF THE INTERVAL THE FUNCTION AND LINEARLY INTERPOLATED VALUES AGREE WITHIN THE USER SPECIFIED FRACTIONAL ALLOWABLE UNCERTAINTY IT IS ASSUMED THAT THE TABULATED VALUES OF THE FUNCTION AT THE ENDS OF THE INTERVAL CAN BE USED TO ACCURATELY REPRESENT THE FUNCTION OVER THE ENTIRE INTERVAL AND THE INTERVAL IS NOT SUB-DIVIDED (I.E., THE PROGRAM WILL INITIALLY ONLY TABULATE THE FUNCTION AT THE ENDS AND MIDPOINT OF THE INTERVAL...SEE, COMMENTS BELOW ON THINNING). NOTE, SINCE EACH X RANGE IS SUB-DIVIDED INTO 100 X INTERVALS IN EACH X RANGE THE PROGRAM WILL CALCULATE THE FUNCTION AT LEAST 200 POINTS (X INTERVAL ENDPOINTS AND MIDPOINT).

IF THE LINEARLY INTERPOLABLE VALUE AND THE FUNCTION DO NOT AGREE AT THE MIDPOINT THE INTERVAL WILL BE DIVIDED IN HALF TO DEFINE A NEW X INTERVAL EXTENDING FROM THE LOWER X LIMIT OF THE PREVIOUS X INTERVAL UP TO THE MIDPOINT OF THE PREVIOUS X INTERVAL. THE TEST FOR CONVERGENCE (DESCRIBED ABOVE) WILL THEN BE APPLIED TO THIS SHORTER X INTERVAL. THE CYCLE OF TESTING FOR CONVERGENCE AND HALVING THE X INTERVAL WILL BE CONTINUED UNTIL EITHER,

(1) THE X INTERVAL BECOMES SHORT ENOUGH TO FORCE CONVERGENCE WHICH WILL ALWAYS OCCUR FOR FUNCTIONS WHICH ARE NOT EQUAL TO 0.0 (SEE, PROOF BELOW).

(2) THE X INTERVAL BECOMES SO SMALL THAT THE X VALUES OF THE TWO

ENDS OF THE INTERVAL ARE IDENTICAL WITHIN THE ACCURACY TO WHICH THEY ARE REPRESENTED IN THE OUTPUT FORMAT (6 DIGITS).

(3) AN INTERVAL IS HALVED 20 TIMES (THE LENGTH OF THE INTERVAL IS REDUCED BY OVER A FACTOR 1.0E+06) AND LINEAR INTERPOLATION FOR SUCCESSIVELY SMALLER INTERVALS IS NOT IMPROVING THE APPROXIMATION OF THE FUNCTION AT THE MIDPOINT.

(4) AN INTERVAL IS HALVED 40 TIMES (THE LENGTH OF THE INTERVAL IS REDUCED BY OVER A FACTOR 1.0E+12).

CASES 2 - 4 WILL ONLY OCCUR CLOSE TO POINTS WHERE A FUNCTION IS 0.0 AND THE HALVING ALGORITHM IS NOT CONVERGING. USUALLY IN THESE CASES THE VALUE OF THE FUNCTION WILL BE QUITE SMALL AND THE DIFFERENCE BETWEEN THE EXACT FUNCTION AND TABULATED VALUE ARE OF LITTLE PRACTICAL CONCERN. IF CASES 2 - 4 OCCUR THE PROGRAM WILL PRINT AN ERROR MESSAGE AND CONTINUE (SEE, BELOW FOR MORE DETAILS).

ONCE CONVERGENCE HAS OCCURRED THE PROGRAM WILL PROCEED TO THE NEXT NEXT X INTERVAL, DEFINED AS EXTENDING FROM THE UPPER X LIMIT OF THE LAST X INTERVAL UP TO THIS VALUE PLUS 1/100 OF THE X RANGE (LOG OR LINEAR SPACED, AS DESCRIBED ABOVE) OR THE UPPER X LIMIT OF THE X RANGE, WHICHEVER IS LESS. THE CYCLE OF CONSIDERING EACH X INTERVAL IS CONTINUED UNTIL THE ENTIRE X RANGE HAS BEEN TABULATED.

X ROUNDING

THE OUTPUT FROM THIS PROGRAM IS A 1 LINE TITLE IDENTIFYING EACH FUNCTIONS, FOLLOWED BY (X,Y) PAIRS, ONE PER LINE. THE (X,Y) PAIRS ARE OUTPUT IN A SPECIAL D11.4 FORMAT TO ALLOW X AND Y TO BE REPRESENTED TO 6 DIGIT ACCURACY (E.G. 1.23456+ 3). WHEN A FUNCTION IS RAPIDLY VARYING (SUCH AS NEAR A THRESHOLD) SMALL SHIFTS IN X MAY RESULT IN LARGE CHANGES IN THE VALUE OF THE FUNCTION. WHEN THE INTERVAL HALVING ALGORITHM IS USED TO OBTAIN TABULATED (X,Y) PAIRS ROUNDING OF X VALUES FROM THEIR BINARY VALUES INSIDE A COMPUTER TO DECIMAL FORM TO THE ACCURACY OF THE OUTPUT FORMAT CAN INTRODUCE SMALL, BUT SIGNIFICANT, SHIFTS IN X WHICH CAN LEAD TO ERRONEOUS RESULTS WHEN THE TABULATED VALUES ARE USED IN APPLICATIONS.

IN ORDER TO AVOID THIS PROBLEM THIS PROGRAM WILL INTERNALLY ROUND ALL X VALUES TO EXACTLY 6 DIGITS ACCURACY BEFORE CALCULATING THE FUNCTION. USING THIS APPROACH THERE WILL BE NO DIFFERENCE BETWEEN THE INTERNAL AND OUTPUT FORMAT VALUES OF X.

THINNING

AFTER CONSTRUCTING A LINEARLY INTERPOLABLE TABLE THE PROGRAM WILL PERFORM A FINAL CHECK AND THIN ALL TABULATED VALUES THAT CAN BE ACCURATELY APPROXIMATED BY LINEAR INTERPOLATION FROM NEIGHBORING TABULATED VALUES. IN ORDER TO MINIMIZE THE FINAL SIZE OF THE TABLE THIS FINAL THINNING IS VERY IMPORTANT (E.G., FOR EACH X RANGE THE PROGRAM WILL PRODUCE AT LEAST 200 TABULATED POINTS...INTERVAL ENDS AND MIDPOINTS...AND WITHOUT THINNING TABLES COULD BECOME EXTREMELY LARGE WHICH COULD NEGATE THE ADVANTAGE OF TABULATING DATA). AFTER THINNING THE TABLE WILL CONTAIN THE MINIMUM NUMBER OF POINTS REQUIRED TO ACCURATELY REPRESENT THE FUNCTION TO THE REQUIRED ACCURACY OVER THE ENTIRE X RANGE.

THE FINAL THINNED RESULTS WILL ALWAYS INCLUDE THE END POINTS OF ALL X RANGES.

TABULATE ONLY AT FIXED X VALUES

IF YOU WOULD LIKE TO OBTAIN A TABLE OF A FUNCTION AT FIXED X VALUES WITHOUT CONSIDERING THE ACCURACY OF INTERPOLATED VALUES (E.G., IF YOU WOULD LIKE A FIXED SIZE TABLE FOR A PUBLICATION). YOU CAN SPECIFY AN ALLOWABLE UNCERTAINTY OF 0.0 FOR ALL X RANGES.

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IF THIS IS DONE THE PROGRAM WILL ONLY TABULATE THE FUNCTION AT THE X VALUES CORRESPONDING TO THE ENDS OF THE X RANGES (UP TO THE 100 X RANGES SPECIFIED BY INPUT). THIS CAN ALSO BE DONE FOR ANY SUBSET OF THE X RANGES (E.G., TABULATE THE FUNCTION AT X = 0.0 AND X = 1.0 WITHOUT SUB-DIVIDING THE INTERVAL AND THEN TABULATE THE FUNCTION ABOVE X = 1.0 TO SOME SPECIFIED UNCERTAINTY).

OPTIMIZING TABLE SIZE

FOR MOST FUNCTIONS THIS PROGRAM HAS A VERY SHORT RUNNING TIME. AS SUCH IT IS POSSIBLE TO OPTIMIZE TABLE SIZE BY PERFORMING A NUMBER OF RUNS USING DIFFERENT ALLOWABLE UNCERTAINTIES IN A NUMBER OF X RANGES. AFTER AN INITIAL RUN TO OBTAIN RESULTS TO HIGH PRECISION (SMALL ALLOWABLE UNCERTAINTY) THE TABULATED VALUES MAY BE EXAMINED TO DETERMINE IF THE PRECISION CAN BE RELAXED IN ONE OR MORE X RANGES IN ORDER TO REDUCE THE SIZE OF THE TABLE. FOR EXAMPLE, NEAR WHERE A FUNCTION IS EQUAL TO 0.0 THIS PROGRAM MAY GENERATE A LARGE NUMBER OF POINTS ON A VERY CLOSELY SPACED X MESH. IF THIS DETAIL IS NOT REQUIRED THE USER MAY SPECIFY X RANGES NEAR THE ZEROES OF THE FUNCTION AND RELAX (OR SET TO 0.0, AS DESCRIBED ABOVE) THE ALLOWABLE UNCERTAINTY.

HOW DOES TABLE SIZE DEPEND ON ACCURACY

AS A ROUGH RULE THE NUMBER OF POINTS IN THE TABLE WILL INCREASE AS PROPORTIONAL TO ONE OVER THE SQUARE ROOT OF THE ACCURACY THAT THE USER SPECIFIES. FOR EXAMPLE, IF A FUNCTION IS TABULATED OVER A GIVEN X RANGE TO 1.0 PER-CENT RESULTING IN A TABLE OF 100 (X,Y) PAIRS, IF THE SAME FUNCTION IS TABULATED OVER THE SAME X RANGE TO 0.1 PER-CENT THE TABLE WILL CONTAIN ABOUT 300 (X,Y) PAIRS.

NOT ALL FUNCTIONS CAN BE REPRESENTED IN TABULATED FORM

THE USER SHOULD BE AWARE OF THE LIMITATIONS OF THIS PROGRAM. NOT ALL FUNCTIONS CAN BE ACCURATELY REPRESENTED IN TABULATED LINEARLY INTERPOLABLE FORM TO WITHIN A USER SPECIFIED UNCERTAINTY.

FORTUNATELY MOST FUNCTIONS OF PHYSICAL INTEREST WHICH ARE EITHER ZERO OR NON-NEGATIVE CAN BE REPRESENTED IN THIS FORM. ALMOST ALL CASES OF PROBABILITIES WHICH ARE INHERENTLY POSITIVE CAN BE TABULATED TO WITHIN A USER SPECIFIED ACCURACY AND THE FOLLOWING COMMENTS ARE INCLUDED ONLY TO INDICATE THE CONVENTIONS THAT HAVE BEEN BUILT INTO THIS PROGRAM TO HANDLE OTHER CASES.

THIS PROGRAM HAS A BUILT-IN SET OF CONVENTIONS WHICH ARE DESIGNED TO INSURE THAT THE PROGRAM CAN PRODUCE A TABLE OF VALUES FOR ANY FUNCTION AND WILL WARN THE USER IF THE TABULATED VALUES CANNOT BE BE USED TO LINEARLY INTERPOLABLE TO APPROXIMATE THE FUNCTION TO WITHIN THE REQUIRED ACCURACY.

THE PROGRAM WILL ATTEMPT TO TABULATE VALUES WHICH ARE WITHIN A USER SPECIFIED FRACTION OF THE EXACT FUNCTION FOR ALL VALUES OF X. THIS INVOLVES TAKING RATIOS OF THE TABULATED VALUES TO THE EXACT VALUES. FOR EXAMPLE, FOR A INTERVAL EXTENDING FROM X = Z TO X = Z + 2*Y IF WE DEFINE.

```
Z+Y         = THE MIDPOINT OF THE INTERVAL.
2*Y         = THE LENGTH OF THE INTERVAL.
F(Z+Y)      = EXACT FUNCTION EVALUATED AT THE MIDPOINT, X = Z + Y
APPROX(Z)   = (F(Z)+F(Z+2*Y))/2
            = APPROXIMATE VALUE OF THE FUNCTION AT THE MIDPOINT
              BASED ON LINEAR INTERPOLATION BETWEEN THE ENDS OF
              THE INTERVAL.
DF(Z,N)     = THE N-TH DERIVATIVE OF F(X) EVALUATED AT X = Z.
```

THE PROGRAM WILL CHECK TO SEE IF,

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ABS((F(Z+Y)-APPROX(Z+Y))/F(Z+Y))
```

IS LESS THAN OR EQUAL TO THE SPECIFIED FRACTIONAL UNCERTAINTY. THE INTERVAL HALVING ALGORITHM WILL CONVERGE IF THIS RATIO BECOMES SMALLER AND APPROACHES 0.0 AS THE LENGTH OF THE INTERVAL (2*Y) APPROACHES 0.0.

IN THE FOLLOWING WE WILL ONLY CONSIDER FUNCTIONS WHICH ARE ANALYTICAL OVER EACH X RANGE. FOR ANY FUNCTION WHICH IS NOT ANALYTICAL THE USER MAY SPECIFY THE POINTS OF DISCONTINUITY AS DIFFERENT X RANGES SO THAT THE FUNCTION IS ANAYTICAL WITHIN EACH X RANGE.

FOR AN ANALYTICAL FUNCTION THE ONLY TIME THAT THE INTERVAL HALVING ALGORITHM DOES NOT CONVERGE IS IF AT SOME X THE FUNCTION AND ITS FIRST DERIVATIVE ARE BOTH 0.0. IN ORDER TO ILLUSTRATE THAT THIS IS TRUE, IF WE CONSIDER AN X INTERVAL EXTENDING FROM Z TO Z + 2*Y WE CAN EXPAND THE ANALYTICAL FUNCTION IN AN INFINITE SERIES ABOUT Z TO DEFINE THE VALUE OF THE FUNCTION AT THE ENDS AND MIDPOINT OF THE INTERVAL,

```
F(Z)          = DF(Z,0)
F(Z+Y)        = (SUM I=0 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!))
              = DF(Z,0)+DF(Z,1)*Y+
              + (SUM I=2 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!))
F(Z+2*Y)      = (SUM I=0 TO INFINITY)*(DF(Z,I)*((2*Y)**I)/(I!))
              = DF(Z,0)
              + (SUM I=1 TO INFINITY)*(DF(Z,I)*((2*Y)**I)/(I!))
```

THE APPROXIMATE VALUE OF THE FUNCTION AT THE MIDPOINT (X = Z + Y) BASED ON LINEAR INTERPOLATION BETWEEN THESE TWO POINTS IS,

```
APPROX(Z+Y)  = (F(Z)+F(Z+2*Y))/2
             = DF(Z,0)+DF(Z,1)*(2*Y)/2+
             + (SUM I=2 TO INFINITY)*(DF(Z,I)*((2*Y)**I)/(I!))/2
```

AND THE DIFFERENCE BETWEEN THE EXACT AND LINEARLY INTERPOLATED VALUES AT THE MIDPOINT IS,

```
F(Z+Y) - APPROX(Z+Y) = (DF(Z,0)+DF(Z,1)*Y) - (DF(Z,0)+DF(Z,1)*Y)
             + (SUM I=2 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!))
             - (SUM I=2 TO INFINITY)*(DF(Z,I)*((2*Y)**I)/(I!))/2
= (SUM I=2 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!)*(1.0-((2**I)/2)))
```

NOTE, THAT THE FIRST 2 TERMS OF THE INFINITE SERIES FOR F(Z+Y) AND APPROX(Z+Y) ARE EXACTLY EQUAL AND CANCEL, SO THAT THE SERIES FOR THE DIFFERENCE ONLY EXTENDS OVER I = 2 TO INFINITY.

IN ORDER TO EXAMINE CONVERGENCE OF THE INTERVAL HALVING TEST WE MUST SEE WHAT HAPPENS AS THE INTERVAL (2*Y) IS MADE PROGRESSIVELY SMALLER. IN THIS CASE THE INTERVAL HALVING TEST IS EQUIVALENT TO,

```
ABS((F(Z+Y)-APPROX(Z+Y))/F(Z+Y)) =
THE ABSOLUTE VALUE OF THE LIMIT AS Y APPROACHES 0.0 OF...
(SUM I=2 TO INFINITY)*(DF(Z,I)*((Y)**I)*(1.0-(2**I)/2))/(I!))/
(SUM I=0 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!)))
```

AS Y APPROACHES 0.0 THE LIMIT OF THE NUMERATOR AND DENOMINATOR OF THIS EXPRESSION WILL APPROACH THE LOWEST ORDER NON-ZERO TERM OF EACH OF THE INFINITE SERIES (SINCE IN EACH CASE THE LOWEST ORDER POWER OF Y WILL BECOME DOMINANT). IF THE LOWER ORDER NON-ZERO TERM OF THE NUMERATOR IS THE N1-TH AND THAT OF THE DENOMINATOR IS THE N2-TH, THE ABOVE RATIO REDUCES TO,

DF(Z,N1)*((Y)**N1)*(1.0-(2**N1)/2)/(N1!))/DF(Z,N2)*(Y**N2)/(N2!))=

(1.0-(2**(N1-1)))*(Y**(N1-N2))*DF(Z,N1)/(N1!)/DF(Z,N2)/(N2!)

NOTE, THAT DF(Z,N1) AND DF(Z,N2) ARE MERELY CONSTANTS DEFINED BY THE DERIVATIVES OF F(X) EVALUATED AT X = Z AND SINCE N1 MUST BE BETWEEN 2 AND INFINITY THE LEADING CONSTANT (1.0-(2**(N1-1)) CANNOT BE ZERO THIS EXPRESSION REDUCES TO,

CONSTANT*(Y**(N1-N2))

AS Y APPROACHES 0.0 THIS RATIO WILL APPROACH 0.0 (I.E. INTERVAL HALVING WILL CONVERGE) ONLY IF N1 IS GREATER THAN N2, SINCE ONLY IN THIS CASE WILL Y**(N1-N2) APPROACH 0.0 AS Y APPROACHES 0.0. THE INFINITE SERIES IN THE NUMERATOR EXTENDS OVER I =2 TO INFINITY SO THAT N1 MUST BE 2 OR MORE, WHEREAS THE INFINITE SERIES IN THE DENOMINATOR EXTENDS OVER I=0 TO FINITY SO THAT N2 MUST BE 0 OR MORE. THEREFORE THIS RATIO WILL DEFINITELY APPROACH 0.0 IF,
(1) N2 = 0 - AT X = Z THE FUNCTION IS NOT EQUAL TO 0.0, OR
(1) N2 = 1 - AT X = Z THE FUNCTION IS EQUAL 0.0 , BUT ITS FIRST DERIVATIVE IS NOT EQUAL TO 0.0.

THE ABOVE PROVES THAT THE ANY FUNCTION WHICH IS EITHER POSITIVE OR NEGATIVE OVER THE ENTIRE X RANGE OR WHOSE FIRST DERIVATIVE IS NOT EQUAL TO 0.0 WHERE THE FUNCTION IS EQUAL TO 0.0 CAN BE TABULATED TO WITHIN A USER SPECIFIED FRACTIONAL ALLOWABLE UNCERTAINTY. IN ANY OTHER CASE CONVERGENCE CANNOT BE GUARANTEED.

AN EXAMPLE OF A SIMPLE FUNCTION WHICH CANNOT BE TABULATED IN LINEAR INTERPOLABLE FORM TO WITHIN A USER SPECIFIED ACCURACY IS (X-Z)**K, (K = 2 OR MORE), IF THE POINT Z IS INCLUDED IN THE X INTERVAL TO BE TABULATED. IN THIS CASE AT X = Z BOTH THE FUNCTION AND ITS FIRST DERIVATIVE (AND ALL DERIVATIVES UP TO ORDER (K-1)) WILL BE EQUAL TO 0.0 AT X = Z. FOR EXAMPLE, IF WE CONSIDER THE SIMPLE FUNCTION F(X) = X*X, FOR SMALL X INTERVALS NEAR X = 0.0 LINEAR INTERPOLATION WILL OVERESTIMATE THE FUNCTION BY A FACTOR OF 2 AND INTERVAL HALVING WILL NOT CONVERGE.

IF A FUNCTION AND ITS FIRST DERIVATIVE ARE BOTH EQUAL TO 0.0 AT X = Z THIS PROGRAM WILL SUB-DIVIDE THE INTERVAL TOWARD X = Z UNTIL ONE OF THE CASES 2 -4, DESCRIBED ABOVE, IS REACHED AT WHICH POINT THE PROGRAM WILL PRINT AN ERROR MESSAGE THAT CONVERGENCE HAS NOT OCCURRED, TABULATE THE FUNCTION AT THE TWO ENDS OF THE THE INTERVAL AND PROCEED TO THE NEXT INTERVAL.

FOR EXAMPLE, IN THE CASE OF X*X LINEARIZED FOR X =0.0 TO 1.0 NEAR X = 0.0 THIS PROGRAM WILL SUB-DIVIDE TO A SMALL INTERVAL FROM 0.0 TO ABOUT 1.0E-08 (F(X) = 1.0E-16) AND THEN STOP SUB-DIVIDING, TABULATE THE FUNCTION AT X = 0.0 AND 1.0E-08, PRINT AN ERROR MESSAGE AND PROCEED TO THE NEXT X INTERVAL FROM 1.0E-08 TO THIS VALUE PLUS 1/100. SINCE X*X IS NOT EQUAL TO 0.0 BETWEEN 1.0E-08 AND 1.0 INTERVAL HALVING WILL CONVERGE FOR ALL OF THE REMAINING X INTERVALS.

WHEN BOTH THE FUNCTION AND ITS FIRST DERIVATIVE ARE EQUAL TO 0.0 AT X = Z FROM THE INFINITE SERIES EXPANSION,

F(Z+Y)   = (SUM I=2 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!))

WE CAN SEE THAT FOR SMALL INTERVALS IN THE VACINITY OF X = Z (SMALL Y) THE VALUE OF THE FUNCTION WILL BE VERY SMALL (DUE TO THE Y**2 AND HIGHER POWERS OF Y) AND OF NO PRACTICAL IMPORTANCE FOR MOST APPLICATIONS.

WHEN THE PROGRAM PRINTS AN ERROR MESSAGE THAT CONVERGENCE HAS NOT OCCURRED IT IS THE USERS RESPONSIBILITY TO VERIFY THAT THE VALUES TABULATED ARE ADEQUATE TO MEET THE NEEDS OF APPLICATIONS.

WHEN CONVERGENCE DOES NOT OCCUR OVER ANY GIVEN INTERVAL AND THE TABULATED RESULTS ARE NOT SATISFACTORY THE USER CAN ALWAYS FORCE THE PROGRAM TO TABULATE THE FUNCTION IN GREATER DETAIL NEAR WHERE THE FUNCTION IS EQUAL TO 0.0 BY SPEFICYING SMALLER X RANGES NEAR EACH 0.0 OF THE FUNCTION. ALTERNATIVELY IF TOO MANY POINTS ARE BEING TABULATED NEAR THE 0.0'S OF A FUNCTION THE USER CAN RELAX (OR SET TO 0.0) THE ALLOWABLE UNCERTAINTY NEAR THE 0.0'S.

FALSE CONVERGENCE

SOME CARE MUST BE EXERCISED IN DEFINING X RANGES IN ORDER TO GUARANTEE THAT THE INTERVAL HALVING METHOD HAS TRULY CONVERGED AND THAT THE METHOD HAS NOT LED TO 'FALSE CONVERGENCE'. THE METHOD WILL ALWAYS CONVERGE IF THE FUNCTION IS EITHER COMPLETELY CONVEX OR CONCAVE WITHIN EACH X INTERVAL. SINCE AN ANALYTICAL FUNCTION WILL ONLY CHANGE FROM CONVEX TO CONCAVE BETWEEN PAIRS OF SUCCESSIVE MAXIMA AND MINIMA THIS PROBLEM CAN ONLY OCCUR IF THERE ARE TOO MANY MAXIMA AND MINIMA IN AN X RANGE. IN PRINCIPLE 'FALSE CONVERGENCE' CAN OCCUR. HOWEVER, IN PRACTICE IF THE INTERVAL HALVING METHOD IS UNDERSTOOD AND A LITTLE CARE IS USED TO DEFINE X RANGES 'FALSE CONVERGENCE' RARELY OCCURS AND THE FOLLOWING SECTION IS INCLUDED HERE ONLY TO EXPLAIN THE POTENTIAL SOURCES OF 'FALSE CONVERGENCE', HOW TO DETECT WHEN IT OCCURS AND WHAT TO DO TO ELIMINATE IT WHEN IT DOES OCCUR.

BY EXAMINING THE INTERVAL HALVING CONVERGENCE TEST,

THE ABSOLUTE VALUE OF,
(SUM I=2 TO INFINITY)*(DF(Z,I)*((Y)**I)*(1.0-(2**I)/2))/(I!))/
(SUM I=0 TO INFINITY)*(DF(Z,I)*((Y)**I)/(I!)))

WE CAN SEE THAT USING AN X INTERVAL WHICH EXTENDS ACROSS AN INFLECTION POINT (I.E., AN X VALUE WHERE THE SECOND DERIVATIVE OF THE FUNCTION, DF(Z,2), IS 0.0 AND THE FUNCTION CHANGES FROM CONVEX TO CONCAVE, OR VICE-VERSA) IF Z IS CLOSE TO THE INFLECTION POINT LINEAR INTERPOLATION BETWEEN POINTS ON EITHER X SIDE OF X = Z MAY INDICATE CONVERGENCE, WHEREAS IN FACT THE FUNCTION CANNOT REALLY BE LINEARLY INTERPOLATED TO WITHIN THE FRACTIONAL ACCURACY OVER THE ENTIRE INTERVAL.

A TRIVIAL EXAMPLE OF FALSE CONVERGENCE OCCURS IF WE TABULATE SIN(X) OVER THE X INTERVAL FROM 0.0 TO 2*PI. THE INTERVAL HALVING METHOD WILL CALCULATE SIN(X) AT THE ENDS OF THE INTERVAL (0.0 AND 2*PI) AND AT THE MIDPOINT OF THE INTERVAL (PI), FIND THAT ALL 3 VALUES ARE EQUAL TO 0.0, SO THAT LINEARLY INTERPOLATION BETWEEN 0.0 AND 2*PI CAN EXACTLY REPRODUCE THE VALUE AT PI AND CONCLUDE THAT THE FUNCTION IS EQUAL TO 0.0 FROM X = 0.0 TO 2*PI.

A MORE SUBTLE CASE OF 'FALSE CONVERGENCE' OCCURS IF WE TABULATE 1 + X**3 OVER THE X INTERVAL FROM -1 TO 1. THE INTERVAL HALVING METHOD WILL CALCULATE 1 + X**3 AT THE ENDS OF THE INTERVAL (-1 AND 1) AND AT THE MIDPOINT OF THE INTERVAL (0 - WHICH IS AN INFLECTION POINT), FIND THAT LINEAR INTERPOLATION BETWEEN X = -1 AND 1 CAN EXACTLY REPRODUCE THE VALUE AT X =0 AND CONCLUDE THAT THE FUNCTION IS LINEAR BETWEEN X = -1 AND 1.

BY DEFINING LOCALS APPROXIMATION TO THE FIRST AND SECOND DERIVATIVES OF THE FUNCTION,

DF(I,1) = (DF(I+1,0)-DF(I,0))/(X(I+1)-X(I))
DF(I,2) = (DF(I+1,1)-DF(I,1))/(X(I+1)-X(I))

THIS PROGRAM CAN APPROXIMATE WHERE THE FUNCTION CHANGES FROM CONVEX TO CONCAVE. WHEN THIS OCCURS THE PROGRAM WILL PRINT AN ERROR MESSAGE. THE USER SHOULD EXAMINE THE TABULATED FUNCTION NEAR ALL SUCH ERROR MESSAGES TO INSURE THAT THE SPACING OF X VALUES ACROSS THE INFLECTION POINT IS NOT LARGE COMPARED TO THE SPACING OF POINTS ON EITHER SIDE OF THE INFLECTION POINT. IF THE X SPACING IS TOO LARGE THE USER SHOULD INSERT THE END OF AN X RANGE NEAR THE INFLECTION POINT AND RE-RUN THE PROGRAM.

SINCE THE FUNCTION SHOULD BE ANALYTICAL WITHIN EACH X RANGE THE FUNCTION SHOULD BE SMOOTH (CONTINUOUS FUNCTION AND SLOPE) AND IF 'FALSE CONVERGENCE' OCCURS IT CAN EASILY BE SEEN BY PLOTTING THE TABULATED RESULTS (SEE, PROGRAM PLOTTAB, WHICH IS DESIGNED TO PLOT THE OUTPUT DATA FROM THIS PROGRAM). WHEN THE TABULATE DATA IS PLOTTED 'FALSE CONVERGENCE' WILL BE INDICATED BY DISTINCT CHANGES IN THE SLOPE OF THE FUNCTION. 'FALSE CONVERGENCE' CAN BE ELIMINATED BY DEFINING SHORTER X RANGES IN THE VACINITY OF THE CHANGES IN THE SLOPE AND RE-RUNNING THIS PROGRAM.

CALCULATING INTEGRALS FROM TABULATED RESULTS

ONE OF THE ADVANTAGES OF TABULATED LINEARLY INTERPOLABLE VALUES IS THE EASE WITH WHICH INTEGRALS MAY BE DEFINED IN A COMPLETELY NUMERICAL STABLE FORM.

```
FOR ANY TABULATED FUNCTION IF WE DEFINE,
DX(I)     = X(I+1) - X(I)
AVF(I)    =(F(I+1) + F(I))/2
DF(I)     =(F(I+1) - F(I))/2
THE INTEGRAL OF ONE FUNCTION IS SIMPLY,

(INTEGRAL X1 TO X2)(F(X)*DX) =
(SUM I)*(DX(I)*AVF(I))

AND THE INTEGRAL OF THE PRODUCT OF TWO FUNCTIONS IS,

(INTEGRAL X1 TO X2)(F(X)*G(X)*DX) =
(SUM I)*(DX(I)*(AVF(I)*AVG(I)+DF(I)*DG(I)/3)
```

THIS SIMPLE ALGORITHM CAN BE EXTENDED TO DEFINE THE INTEGRAL OF THE PRODUCT OF ANY NUMBER OF TABULATED FUNCTIONS.

FOR FUNCTIONS WHICH DO NOT CHANGE SIGNS BETWEEN X1 AND X2 THIS SUM CAN BE CALCULATED IN A COMPLETELY NUMERICAL STABLE MANNER WITHOUT ROUND-OFF PROBLEMS AND IF THE TABULATED VALUES OF F(I) AND G(I) CAN ACCURATELY REPRESENT THE FUNCTIONS F(X) AND G(X) TO A GIVEN ACCURACY THE RESULTING INTEGRALS ARE GUARANTEED TO BE CORRECT TO WITHIN THE GIVEN ACCURACY.

USER DEFINED FUNCTION

THIS PROGRAM IS DISTRIBUTED WITH AN EXAMPLE FUNCTION IN ORDER TO ILLUSTRATE HOW THIS PROGRAM WORKS. IN ORDER TO CALCULATE RESULTS FOR ANY OTHER FUNCTION THE USER NEED ONLY,

(1) REPLACE THE DOUBLE PRECISION FUNCTION FUNKY(X) BY ANY OTHER FUNCTION (IT MUST STILL BE A DOUBLE PRECISION FUNCTION NAMED FUNKY AND MUST BE A FUNCTION OF A SINGLE CONTINUOUS VARIABLE X).
(2) PREPARE INPUT (AS DESCRIBED BELOW) TO DEFINE X RANGES, ALLOWABLE UNCERTAINTIES AND CONSTANTS FOR EACH X RANGE.
(3) DESIGN THE DOUBLE PRECISION FUNCTION TO PROPERLY INTERPRET THE CONSTANTS WHEN THE FUNCTION IS CALLED.

THE USER SUPPLIED FUNCTION MUST BE A DOUBLE PRECISION FUNCTION

OF A SINGLE VARIABLE, X, NAMED FUNKY, E.G.,

```
DOUBLE PRECISION FUNCTION FUNKY(X)
DOUBLE PRECISION XRANGE,CON,ERROK
COMMON/FUNCOM/XRANGE(100),CON(50,100),ERROK(100),NCON(100),
1 IRANGE,NRANGE,MODEL
       .
       .
(ANY REQUIRED CALCULATIONS)
       .
       .
FUNKY=(RESULT OF CALCULATIONS)
RETURN
END
```

LABELLED COMMON INTERFACE

THE PROGRAM WILL READ THE FOLLOWING PARAMETERS AS INPUT AND STORE THEM IN LABELLED COMMON/FUNCOM/.

```
XRANGE = X LIMIT OF EACH X RANGE (NRANGE+1 VALUES).
CON    = COEFFICENTS IN EACH X RANGE (0 TO 50 IN EACH X RANGE).
ERROK  = ALLOWABLE FRACTIONAL UNCERTAINTY IN EACH X RANGE
         (E.G., 0.001 = 0.1 PER-CENT)
NCON   = THE NUMBER OF COEFFICIENTS IN EACH X RANGE
IRANGE = INDEX TO CURRENT X RANGE
NRANGE = THE NUMBER OF X RANGES (1 TO 100)
MODEL  = MODEL NUMBER
```

ONCE READ ALL OF THIS INFORMATION WILL NOT BE CHANGED BY THE PROGRAM AND IS MERELY PASSED TO THE USER SUPPLIED FUNCTION. THE ONLY EXCEPTION BEING THE INDEX TO THE CURRENT X RANGE (IRANGE) WHICH WILL BE DEFINED BY THE PROGRAM BEFORE CALLING THE FUNCTION. WHEN THERE IS MORE THAN ONE X RANGE THIS PARAMETER MAY BE USED BY THE FUNCTION TO DEFINE WHICH COEFFICIENTS TO USE WHEN THE FUNCTION IS CALLED.

FOR AN EXAMPLE SEE THE BELOW EXAMPLE INPUT AND THE FUNCTION SUPPLIED WITH THIS PROGRAM.

DEFINITION OF VARIABLES

```
TITLES= 1 LINE DESCRIPTION OF PROBLEM
NRANGE= NUMBER OF X RANGES
MODEL = MODEL NUMBER
NCON  = NUMBER OF COEFFICIENTS IN EACH X RANGE
XRANGE= X LIMIT OF EACH RANGE.
ERROK = ALLOWABLE FRACTIONAL UNCERTAINTY (E.G. 0.001=0.1 PER-CENT)
CON   = COEFFICENTS IN EACH RANGE
IRANGE= INDEX TO CURRENT X RANGE
```

I/O UNITS

UNIT	DESCRIPTION
5	INPUT PARAMETERS
6	OUTPUT REPORT
10	TABULATED OUTPUT

INPUT DATA FORMAT

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-72	18A4	PHYSICAL DESCRIPTION OF DATA
2	1-11	I11	NUMBER OF X RANGES (1 TO 100).

			NOTE, N RANGES ARE DEFINED BY N+1 X VALUES. SEE, EXAMPLE INPUT BELOW
	12-22	I11	MODEL NUMBER
3	1-11	I11	NUMBER OF COEFFICENTS IN X RANGE (0-50).
	12-22	D11.4	LOWER X LIMIT OF RANGE.
	23-33	D11.4	ALLOWABLE FRACTIONAL UNCERTAINTY IN X RANGE (E.G., 0.001 = 0.1 PER-CENT)
4-N	1-66	6D11.4	COEFFICENTS IN X RANGE (0 TO 50 PER X RANGE).

LINES 3 AND 4-N ARE REPEATED FOR EACH RANGE (UP TO THE NUMBER OF RANGES DEFINED ON LINE 2, COLUMNS 1-11). IF THE NUMBER OF COEFFICIENTS IN ANY ENERGY RANGE IS ZERO CARDS 4-N ARE NOT INPUT (SEE, EXAMPLE INPUT NO. 2 BELOW). AFTER CARDS 3 AND 4-N ARE READ FOR EACH X RANGE A FINAL LINE 3 IS READ TO SPECIFY THE UPPER X LIMIT OF THE LAST X RANGE.

THE INPUT MAY BE REPEATED FOR ANY NUMBER OF CASES. EXECUTION TERMINATES AT THE END OF THE INPUT DATA.

EXAMPLE MODELS

AS DISTRIBUTED THIS PROGRAM HAS TWO BUILT-IN EXAMPLE MODELS,
(1) THE BELFAST MODEL FOR IONIZATION CROSS SECTIONS,
(2) A REACTION WEIGHTING FUNCTION = SQRT(X)*MAXWELLIAN(X)
THE FOLLOWING EXAMPLE INPUTS USE EACH OF THESE TWO MODELS.

EXAMPLE INPUT NO. 1

USE THE BELFAST MODEL FOR IONIZATION CROSS SECTIONS,

SIGMA(E)=(-A*LOG(X) + SUM(J=1 TO N) B(J)*(1-X)**J)/(E*ION)

```
E      = ENERGY (EV)
ION    = IONIZATION POTENTIAL (EV) (CON(1,IRANGE))
A      = COEFFICIENT IN EACH E RANGE (CON(2,IRANGE))
B      = COEFFICIENTS IN EACH E RANGE (CON(J,IRANGE),J=3 TO NCON)
X      = ION/E
```

NOTE, THE COEFFICIENT TABLE IN EACH E RANGE (CON) IS INTERPRETED TO CONTAIN,

```
CON(1,IRANGE)              = ION
CON(2,IRANGE)              = A
CON(3 THROUGH NCON,IRANGE) = B
NCON                       = NUMBER OF COEFFICIENTS READ FOR EACH
                             E RANGE.
```

INSURE THAT IN EACH ENERGY RANGE NCON IS 2 + THE NUMBER OF B COEFFICIENTS, NOT THE NUMBER OF B COEFFICIENTS.

USE 2 ENERGY RANGES, 138.1 TO 405.3 EV AND 405.3 TO 12000 EV. CALCULATE THE CROSS SECTIONS IN BOTH RANGES USING A FRACTIONAL UNCERTAINTY OF 0.001 (0.1 PER-CENT). THE FIRST ENERGY RANGE HAS 5 B COEFFICIENTS. IN THIS RANGE THE DATA INPUT INCLUDES,

```
ION    = 138.1 EV
A      = 0.336
B      = 0.08, 0.143, -0.731, 1.336 AND -0.785
```

THE SECOND ENERGY RANGE HAS 3 B COEFFICIENTS. IN THIS RANGE THE DATA INPUT INCLUDES,

```
ION    = 320.0 EV
A      = 0.801
```


THE REQUIRED INTEGRAL IS SIMPLY

```
B     = 3.865, -4.605, 1.543

FOLLOWING 8 INPUT LINES ARE REQUIRED,

BELFAST RECOMMENDATION                                 O VI -> VII
          2          1
          7 1.3810D+02 1.0000D-03
 1.3810D+02 0.3360D+00 0.0800D+00 0.1430D+00-0.7310D+00 1.3360D+00
-0.7850D+00
          5 4.4053D+02 1.0000D-03
 3.2000D+02 0.8010D+00 3.8650D+00-4.6050D+00 1.5430D+00
            1.2000D+04
```

NOTE, THE LAST INPUT LINE ONLY DEFINES THE UPPER X LIMIT OF THE LAST X RANGE.

EXAMPLE INPUT NO. 2
===

CALCULATE A REACTION WEIGHTING FUNCTION = SQRT(X)*MAXWELLIAN(X),

SQRT(X)*MAXWELL = X*DEXP(-X), FOR X=0.0 TO 50.0

USE THE X RANGES 0.0 TO 1.0 (UP TO PEAK), 1.0 TO 2.0 (UP TO THE INFLECTION POINT), 2.0 TO 5.0 AND 5.0 TO 50.0. TREAT THE X RANGE UP TO 5.0 VERY PRECISELY USING AN ALLOWABLE FRACTIONAL UNCERTAINTY OF 0.0001 (0.01 PER-CENT). FOR THE X RANGE ABOVE 5.0 0.001 (0.1 PER-CENT). IN THIS CASE NO COEFFICIENTS ARE NECESSARY FOR EACH RANGE. THE FOLLOWING 6 INPUT LINES ARE REQUIRED,

```
REACTION WEIGHTING
          4          2
          0 0.0000D+00 1.0000D-04
          0 1.0000D+00 1.0000D-04
          0 2.0000D+00 1.0000D-04
          0 5.0000D+00 1.0000D-03
            5.0000D+01
```

EXAMPLE INPUT NO. 3
===

RUN BOTH OF THE ABOVE EXAMPLE INPUTS ONE AFTER THE OTHER,

```
BELFAST RECOMMENDATION                                 O VI -> VII
          2          1
          7 1.3810D+02 1.0000D-03
 1.3810D+02 0.3360D+00 0.0800D+00 0.1430D+00-0.7310D+00 1.3360D+00
-0.7850D+00
          5 4.4053D+02 1.0000D-03
 3.2000D+02 0.8010D+00 3.8650D+00-4.6050D+00 1.5430D+00
            1.2000D+04
REACTION WEIGHTING
          4          2
          0 0.0000D+00 1.0000D-04
          0 1.0000D+00 1.0000D-04
          0 2.0000D+00 1.0000D-04
          0 5.0000D+00 1.0000D-03
            5.0000D+01
```

OUTPUT TABULATED CROSS SECTIONS FORMAT
===

THE PROGRAM WILL OUTPUT THE (X,Y) PAIRS DESCRIBING THE FUNCTION ON UNIT 10 (AS DESCRIBED BELOW). IN ADDITION THE PROGRAM WILL OUTPUT ON UNIT 6 A LISTING PRESENTING NOT ONLY THE X VALUE AND THE VALUE OF THE FUNCTION (Y), BUT ALSO THE LOCAL APPROXIMATION TO THE FIRST AND SECOND DERIVATIVES (DESCRIBED ABOVE) AND WARNING AND/OR ERROR MESSAGES. THE USER SHOULD CAREFULLY CHECK THIS LISTING AND IF

NECESSARY TAKE CORRECTIVE ACTION BEFORE USING THE TABULATED DATA IN ANY APPLICATION.

THE FORMAT OF THE DATA ON UNIT 10 WILL BE,

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-72	18A4	PHYSICAL DESCRIPTION OF DATA
2-N	1-11	D11.4	X
	12-22	D11.4	Y

THE TABLE OF X VS. Y IS TERMINATED BY A BLANK LINE (NOT 0.0), WHICH MAY BE USED TO FIND THE END OF THE DATA FOR EACH CASE. THE OUTPUT IS REPEATED FOR EACH CASE. FOR EXAMPLE, THE OUTPUT CORRESPONDING TO THE EXAMPLE INPUT NO. 1 DESCRIBED ABOVE WOULD LOOK LIKE,

```
BELFAST RECOMMENDATION                                O VI -> VII
 1.38100+ 2 0.00000+ 0
 1.38289+ 2 2.97987-21
 1.38667+ 2 8.90933-21
 1.39234+ 2 1.77261-20
     .          .
     .          .
     .          .
     .          .
 1.03430+ 4 1.09047-19
 1.10497+ 4 1.03530-19
 1.19023+ 4 9.76384-20
 1.20000+ 4 9.70099-20
                      (BLANK LINE TERMINATES CURVE)
```

Example LINTAB output

The following page illustrates the results obtained using program LINTAB for the example problem distributed with this program. The plot was produced using program PLOTTAB.

TO MEET THE NEEDS OF ANY APPLICATION. IN PARTICULAR WHEN DEALING
WITH PHYSICAL DATA WHICH HAS AN INHERENT UNCERTAINTY ASSOCIATED

LINEARLY INTERPOLABLE TABLES FROM FUNCTIONS (LINTAB 87-1)

PROBLEM DESCRIPTION

O I -> II (q = 0) Belfast Recommendation

NUMBER OF X RANGES.................... 1
MODEL NUMBER.......................... 1

RANGE................................. 1
NUMBER OF COEFFICIENTS................ 4
LOWER X LIMIT OF RANGE................ 1.3600D+01
ALLOWABLE FRACTIONAL UNCERTAINTY...... 1.0000D-03 (0.1000 PER-CENT)
COEFFICIENTS.......................... 1.3600D+01
2.4550D+00
-2.1810D+00
-1.5700D+00

UPPER X LIMIT OF LAST RANGE.......... 1.0000D+06

TABULATED RESULTS

POINT	X	FUNCTION	FIRST DERIVATIVE	SECOND DERIVATIVE	
1	1.36000+ 1	0.00000+ 0			END OF RANGE
2	1.36062+ 1	6.74346-20	1.08765-17	-3.87283-18	
3	1.36187+ 1	2.02786-19	1.06281-17	-5.16297-18	
4	1.36311+ 1	3.36261-19	1.07641-17	-3.81992-18	
5	1.36558+ 1	5.99804-19	1.06698-17	-4.20994-18	
6	1.36920+ 1	9.80532-19	1.05173-17	-4.94795-18	
7	1.37275+ 1	1.34766-18	1.03417-17	-4.21290-18	
8	1.37739+ 1	1.81845-18	1.01462-17	-4.71926-18	
9	1.38188+ 1	2.26450-18	9.93433-18	-3.79324-18	
10	1.38837+ 1	2.89326-18	9.68815-18	-5.55884-18	
11	1.39252+ 1	3.28574-18	9.45745-18	-3.15391-18	
12	1.40056+ 1	4.02574-18	9.20388-18	-4.11415-18	
13	1.40810+ 1	4.69632-18	8.89367-18	-3.24437-18	
14	1.41848+ 1	5.58453-18	8.55691-18	-3.69275-18	
15	1.42801+ 1	6.36646-18	8.20499-18	-2.99397-18	
16	1.43966+ 1	7.28171-18	7.85619-18	-2.72685-18	
17	1.45432+ 1	8.37482-18	7.45644-18	-3.05585-18	
18	1.46659+ 1	9.24372-18	7.08148-18	-2.40935-18	
19	1.48025+ 1	1.01661-17	6.75237-18	-2.23570-18	
20	1.49489+ 1	1.11067-17	6.42506-18	-1.90668-18	
21	1.51247+ 1	1.21773-17	6.08986-18	-1.72818-18	
22	1.53253+ 1	1.33294-17	5.74319-18	-1.56270-18	
23	1.55366+ 1	1.44732-17	5.41299-18	-1.21064-18	
24	1.58079+ 1	1.58526-17	5.08455-18	-1.06620-18	
25	1.61100+ 1	1.72913-17	4.76245-18	-7.75476-19	
26	1.65065+ 1	1.90577-17	4.45497-18	-5.70222-19	
27	1.70164+ 1	2.11811-17	4.16422-18	-4.33658-19	
28	1.75208+ 1	2.31712-17	3.94548-18	-1.60103-19	
29	1.86557+ 1	2.74427-17	3.76378-18	-2.64183-20	
					WARNING...INFLECTION POINT
30	2.12910+ 1	3.71779-17	3.69416-18	1.22846-20	
					WARNING...INFLECTION POINT
31	2.52275+ 1	5.19103-17	3.74252-18	-4.45327-20	
32	2.74291+ 1	5.99340-17	3.64447-18	-7.66111-20	
33	2.97982+ 1	6.81381-17	3.46297-18	-1.17467-19	
34	3.15648+ 1	7.38892-17	3.25546-18	-1.10565-19	
35	3.33315+ 1	7.92955-17	3.06012-18	-1.07948-19	
36	3.53076+ 1	8.49211-17	2.84681-18	-1.13442-19	
37	3.72837+ 1	9.01037-17	2.62263-18	-1.03999-19	
38	3.94941+ 1	9.53927-17	2.39275-18	-1.04074-19	

THE (X,Y) ONCE. IF THE FUNCTION IS DISCONTINUOUS THE PROGRAM WILL


```
 39 4.17046+ 1 1.00173-16 2.16270-18-9.16067-20
 40 4.41771+ 1 1.04961-16 1.93620-18-8.86490-20
 41 4.66497+ 1 1.09206-16 1.71700-18-7.57769-20
 42 4.94154+ 1 1.13375-16 1.50743-18-7.15132-20
 43 5.21811+ 1 1.16997-16 1.30964-18-5.97511-20
 44 5.52747+ 1 1.20477-16 1.12480-18-5.52592-20
 45 5.83684+ 1 1.23428-16 9.53844-19-4.53031-20
 46 6.18289+ 1 1.26186-16 7.97073-19-3.28687-20
 47 6.72248+ 1 1.29530-16 6.19716-19-3.11075-20
 48 7.30310+ 1 1.32080-16 4.39100-19-2.35511-20
 49 7.95257+ 1 1.33938-16 2.86142-19-1.81294-20
 50 8.65338+ 1 1.35053-16 1.59090-19-1.76928-20
 51 9.13770+ 1 1.35408-16 7.34004-20-7.63496-21
 52 1.02212+ 2 1.35307-16-9.32436-21-6.84885-21
 53 1.14332+ 2 1.34188-16-9.23325-20-4.12170-21
 54 1.27689+ 2 1.32179-16-1.48210-19-1.69498-21
 55 1.51534+ 2 1.27727-16-1.88288-19-2.63029-22
                                                WARNING...INFLECTION POINT
 56 2.12082+ 2 1.15362-16-2.04214-19 4.52446-22
 57 2.50507+ 2 1.08183-16-1.86829-19 5.90593-22
 58 2.80211+ 2 1.03155-16-1.69286-19 4.69615-22
 59 3.13437+ 2 9.80485-17-1.53682-19 4.24698-22
 60 3.50602+ 2 9.29235-17-1.37899-19 3.69678-22
 61 3.92174+ 2 8.78296-17-1.22530-19 3.13097-22
 62 4.38676+ 2 8.28088-17-1.07971-19 3.05587-22
 63 4.77687+ 2 7.90618-17-9.60495-20 2.27171-22
 64 5.1978[illegible]+ 2 7.54211-17-8.64867-20 1.93790-22
 65 5.65144+ 2 7.18967-17-7.76960-20 1.64478-22
 66 6.13956+ 2 6.84961-17-6.96675-20 1.36089-22
 67 6.68555+ 2 6.50980-17-6.22371-20 1.16027-22
 68 7.27470+ 2 6.18340-17-5.54014-20 9.68135-23
 69 7.90957+ 2 5.87070-17-4.92550-20 8.05978-23
 70 8.59273+ 2 5.57182-17-4.37489-20 6.55497-23
 71 9.35688+ 2 5.27579-17-3.87399-20 5.50319-23
 72 1.01814+ 3 4.99379-17-3.42024-20 4.52796-23
 73 1.10700+ 3 4.72562-17-3.01789-20 3.72309-23
 74 1.20261+ 3 4.47111-17-2.66192-20 2.99344-23
 75 1.30956+ 3 4.22066-17-2.34177-20 2.48708-23
 76 1.42496+ 3 3.98354-17-2.05476-20 2.02685-23
 77 1.54932+ 3 3.75935-17-1.80270-20 1.65190-23
 78 1.68314+ 3 3.54770-17-1.58165-20 1.31756-23
 79 1.83282+ 3 3.34048-17-1.38443-20 1.08639-23
 80 1.99434+ 3 3.14521-17-1.20896-20 8.79261-24
 81 2.16838+ 3 2.96143-17-1.05593-20 7.11928-24
 82 2.35567+ 3 2.78864-17-9.22596-21 5.64431-24
 83 2.56516+ 3 2.62013-17-8.04353-21 4.62785-24
 84 2.79121+ 3 2.46196-17-6.99741-21 3.72540-24
 85 3.03480+ 3 2.31361-17-6.08994-21 3.00171-24
 86 3.29692+ 3 2.17461-17-5.30313-21 2.99942-24
 87 3.49238+ 3 2.08241-17-4.71686-21 2.16282-24
 88 3.68785+ 3 1.99847-17-4.29410-21 1.76614-24
 89 3.90649+ 3 1.91303-17-3.90795-21 1.61183-24
 90 4.12513+ 3 1.83529-17-3.55554-21 1.31509-24
 91 4.36969+ 3 1.75620-17-3.23392-21 1.19924-24
 92 4.61426+ 3 1.68429-17-2.94062-21 9.77738-25
 93 4.88782+ 3 1.61116-17-2.67315-21 8.90956-25
 94 5.16139+ 3 1.54470-17-2.42941-21 7.25871-25
 95 5.46739+ 3 1.47715-17-2.20729-21 6.61000-25
 96 5.77340+ 3 1.41580-17-2.00502-21 5.38168-25
 97 6.11568+ 3 1.35347-17-1.82082-21 4.89760-25
 98 6.45797+ 3 1.29689-17-1.65318-21 3.98495-25
 99 6.84084+ 3 1.23943-17-1.50061-21 3.62440-25
100 7.22372+ 3 1.18729-17-1.36184-21 2.94728-25
101 7.65199+ 3 1.13437-17-1.23561-21 2.67916-25
102 8.08026+ 3 1.08637-17-1.12087-21 2.17739-25
```

(SEE, PROOF BELOW).
(2) THE X INTERVAL BECOMES SO SMALL THAT THE X VALUES OF THE TWO

103	8.55931+ 3	1.03767-17-1.01656-21	1.97827-25
104	9.03837+ 3	9.93513-18-9.21795-22	1.60695-25
105	9.57423+ 3	9.48732-18-8.35585-22	1.45927-25
106	1.01101+ 4	9.08141-18-7.57487-22	1.18479-25
107	1.07095+ 4	8.66994-18-6.86471-22	1.07541-25
108	1.13089+ 4	8.29710-18-6.22010-22	8.72768-26
109	1.19793+ 4	7.91933-18-5.63500-22	7.91758-26
110	1.26498+ 4	7.57710-18-5.10413-22	6.42342-26
111	1.33997+ 4	7.23047-18-4.62243-22	5.82473-26
112	1.41497+ 4	6.91655-18-4.18558-22	4.72328-26
113	1.49886+ 4	6.59866-18-3.78934-22	4.28184-26
114	1.58275+ 4	6.31091-18-3.43014-22	3.47063-26
115	1.67658+ 4	6.01961-18-3.10449-22	3.14488-26
116	1.77042+ 4	5.75598-18-2.80937-22	2.54825-26
117	1.87538+ 4	5.48918-18-2.54191-22	2.30826-26
118	1.98035+ 4	5.24779-18-2.29961-22	1.86966-26
119	2.09776+ 4	5.00357-18-2.08010-22	1.69310-26
120	2.21517+ 4	4.78268-18-1.88131-22	1.37084-26
121	2.34650+ 4	4.55925-18-1.70128-22	1.24101-26
122	2.47783+ 4	4.35723-18-1.53829-22	1.00448-26
123	2.62473+ 4	4.15293-18-1.39074-22	9.09043-27
124	2.77164+ 4	3.96824-18-1.25719-22	7.35600-27
125	2.93596+ 4	3.78152-18-1.13631-22	6.65522-27
126	3.10028+ 4	3.61277-18-1.02696-22	5.38360-27
127	3.28408+ 4	3.44220-18-9.28005-23	4.86933-27
128	3.46789+ 4	3.28808-18-8.38502-23	3.93795-27
129	3.67349+ 4	3.13233-18-7.57538-23	3.56092-27
130	3.87909+ 4	2.99163-18-6.84325-23	2.87892-27
131	4.10907+ 4	2.84947-18-6.18116-23	2.60266-27
132	4.33905+ 4	2.72109-18-5.58260-23	2.10366-27
133	4.59630+ 4	2.59139-18-5.04143-23	1.90132-27
134	4.85355+ 4	2.47429-18-4.55232-23	1.53642-27
135	5.14130+ 4	2.35601-18-4.11021-23	1.38831-27
136	5.42905+ 4	2.24924-18-3.71073-23	1.12160-27
137	5.75092+ 4	2.14142-18-3.34972-23	1.01326-27
138	6.07279+ 4	2.04410-18-3.02358-23	8.18428-28
139	6.43282+ 4	1.94585-18-2.72892-23	7.39196-28
140	6.79286+ 4	1.85718-18-2.46278-23	5.96944-28
141	7.19558+ 4	1.76768-18-2.22238-23	5.39040-28
142	7.59831+ 4	1.68692-18-2.00529-23	4.35212-28
143	8.04879+ 4	1.60542-18-1.80923-23	3.92927-28
144	8.49927+ 4	1.53189-18-1.63223-23	3.17175-28
145	9.00316+ 4	1.45770-18-1.47241-23	2.86301-28
146	9.50706+ 4	1.39077-18-1.32814-23	2.31065-28
147	1.00707+ 5	1.32326-18-1.19790-23	2.08544-28
148	1.06343+ 5	1.26237-18-1.08037-23	1.68261-28
149	1.12648+ 5	1.20094-18-9.74278-24	1.51851-28
150	1.18952+ 5	1.14555-18-8.78551-24	1.22485-28
151	1.26005+ 5	1.08968-18-7.92163-24	1.10525-28
152	1.33057+ 5	1.03932-18-7.14220-24	8.91410-29
153	1.40946+ 5	9.88520-19-6.43897-24	8.04183-29
154	1.48834+ 5	9.42733-19-5.80463-24	6.48503-29
155	1.57658+ 5	8.96562-19-5.23239-24	5.84909-29
156	1.66482+ 5	8.54946-19-4.71627-24	4.71657-29
157	1.76352+ 5	8.12991-19-4.25074-24	4.25317-29
158	1.86222+ 5	7.75179-19-3.83095-24	3.42898-29
159	1.97263+ 5	7.37062-19-3.45236-24	3.09190-29
160	2.08303+ 5	7.02716-19-3.11101-24	2.49224-29
161	2.20653+ 5	6.68096-19-2.80322-24	2.24694-29
162	2.33002+ 5	6.36906-19-2.52575-24	1.81093-29
163	2.46816+ 5	6.05471-19-2.27559-24	1.63237-29
164	2.60630+ 5	5.77151-19-2.05009-24	1.31552-29
165	2.76082+ 5	5.48614-19-1.84682-24	1.18562-29
166	2.91534+ 5	5.22908-19-1.66361-24	9.55361-30
167	3.08818+ 5	4.97008-19-1.49849-24	8.60908-30

YOU CAN SPECIFY AN ALLOWABLE UNCERTAINTY OF 0.0 FOR ALL X RANGES.

168	3.26102+ 5	4.73680-19	-1.34969-24	6.93608-30	
169	3.45436+ 5	4.50178-19	-1.21559-24	6.24983-30	
170	3.64769+ 5	4.29013-19	-1.09476-24	5.03455-30	
171	3.86395+ 5	4.07692-19	-9.85884-25	4.53577-30	
172	4.08021+ 5	3.88492-19	-8.87793-25	3.65342-30	
173	4.32212+ 5	3.69154-19	-7.99413-25	3.29115-30	
174	4.56402+ 5	3.51742-19	-7.19800-25	2.65055-30	
175	4.83461+ 5	3.34206-19	-6.48079-25	2.38745-30	
176	5.10519+ 5	3.18418-19	-5.83479-25	1.92254-30	
177	5.40786+ 5	3.02519-19	-5.25290-25	1.73147-30	
178	5.71053+ 5	2.88206-19	-4.72883-25	1.39419-30	
179	6.04909+ 5	2.73794-19	-4.25681-25	1.25548-30	
180	6.38765+ 5	2.60821-19	-3.83176-25	1.01080-30	
181	6.76636+ 5	2.47760-19	-3.44896-25	9.10158-31	
182	7.14506+ 5	2.36004-19	-3.10428-25	7.32692-31	
183	7.56867+ 5	2.24169-19	-2.79390-25	6.59664-31	
184	7.99228+ 5	2.13517-19	-2.51446-25	5.30996-31	
185	8.46612+ 5	2.02795-19	-2.26286-25	4.78026-31	
186	8.93995+ 5	1.93146-19	-2.03635-25	3.84739-31	
187	9.46998+ 5	1.83434-19	-1.83243-25	3.46330-31	
188	1.00000+ 6	1.74694-19			END OF RANGE...NO CONVERGENCE

END OF TABLE

PROBLEM DESCRIPTION

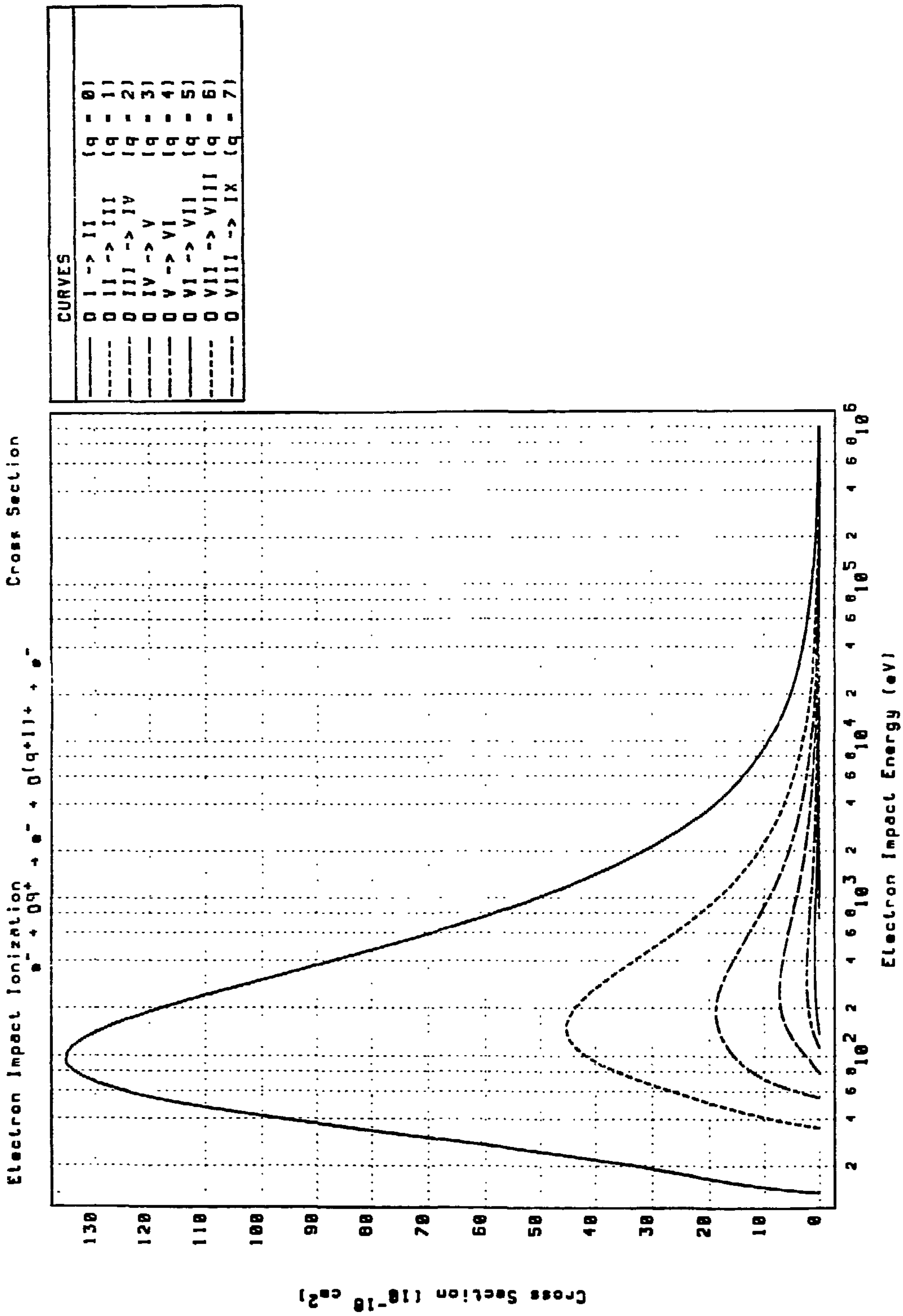
O II -> III (q = 1) Belfast Recommendation

NUMBER OF X RANGES....................	1
MODEL NUMBER..........................	1
RANGE.................................	1
NUMBER OF COEFFICIENTS................	6
LOWER X LIMIT OF RANGE................	3.5100D+01
ALLOWABLE FRACTIONAL UNCERTAINTY.....	1.0000D-03 (0.1000 PER-CENT)
COEFFICIENTS..........................	3.5100D+01
	1.5260D+00
	-5.9300D-01
	-3.9900D-01
	-5.8300D-01
	3.2350D+00
UPPER X LIMIT OF LAST RANGE..........	1.0000D+06

TABULATED RESULTS

POINT	X	FUNCTION	FIRST DERIVATIVE	SECOND DERIVATIVE	
1	3.51000+ 1	0.00000+ 0			END OF RANGE
2	3.51296+ 1	6.37768-20	2.15462-18	-1.48310-19	
3	3.51883+ 1	1.89742-19	2.14591-18	-1.97810-19	
4	3.52461+ 1	3.13115-19	2.13448-18	-1.46858-19	
5	3.53600+ 1	5.54327-19	2.11775-18	-1.63403-19	
6	3.55237+ 1	8.96625-19	2.09100-18	-1.93979-19	
7	3.56807+ 1	1.22013-18	2.06055-18	-1.66259-19	
8	3.58813+ 1	1.62679-18	2.02720-18	-1.56683-19	
9	3.61604+ 1	2.18037-18	1.98347-18	-1.63134-19	
10	3.64910+ 1	2.81828-18	1.92954-18	-1.79517-19	
11	3.67910+ 1	3.38098-18	1.87568-18	-1.45893-19	
12	3.71760+ 1	4.08149-18	1.81951-18	-1.48602-19	
13	3.76048+ 1	4.83438-18	1.75579-18	-1.74048-19	
14	3.79264+ 1	5.38104-18	1.69982-18	-1.17770-19	
15	3.84089+ 1	6.17378-18	1.64299-18	-1.33419-19	
16	3.88914+ 1	6.93547-18	1.57862-18	-1.19575-19	

DF(Z,N) = THE N-TH DERIVATIVE OF F(X) EVALUATED AT X = Z.



OF THE NUMERATOR IS THE N1-TH AND THAT OF THE
N2-TH, THE ABOVE RATIO REDUCES TO,

Program HEATER

FOR MOST APPLICATIONS.


```
 PROGRAM HEATER(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10,
1 TAPE11,TAPE12)

 PROGRAM HEATER
 VERSION 87-1 (JULY, 1987)

 WRITTEN BY DERMOTT E. CULLEN
            NUCLEAR DATA SECTION
            INTERNATIONAL ATOMIC ENERGY AGENCY
            P.O. BOX 100
            VIENNA, AUSTRIA
 TELEPHONE  23-60-1718

 PURPOSE
 ==================================================================
 CALCULATE A LINEARLY INTERPOLATE TABLE OF SPECTRUM AVERAGED
 REACTION RATES STARTING FROM TABULATED LINEAR INTERPOLABLE ENERGY
 DEPENDENT CROSS SECTIONS AND A WEIGHTING SPECTRUM WHICH IS EITHER
 (1) V*MAXWELLIAN.
 (2) A GENERAL LINEARLY INTERPOLABLE TABULATED WEIGHTING SPECTRUM.

 THIS PROGRAM WILL USE THE INTERVAL HALVING ALGORITHM WHICH IS
 DESCRIBED IN DETAIL IN THE DOCUMENATION FOR PROGRAM LINTAB AND
 WILL NOT BE REPEATED HERE (SEE, PROGRAM LINTAB DOCUMENTATION FOR
 DETAILS).

 PARTICLE CROSS SECTIONS
 ==================================================================
 AS DISTRIBUTED THIS PROGRAM ASSUMES THAT THE CROSS SECTIONS ARE
 FOR ELECTRONS. THIS IS DEFINED BY THE PARAMETER AMUMAS WHICH IS
 THE ELECTRON MASS. TO USE THIS PROGRAM FOR ANY OTHER PARTICLE
 ONE NEED ONLY RE-DEFINE AMUMAS (THIS IS MERELY A RE-NORMALIZATION
 FACTOR FOR THE SPECTRUM).

 UNITS OF RESULTS
 ==================================================================
 THE OUTPUT LISTING IDENTIFIES THE REACTION RATES AS BEING IN UNITS
 OF CM**3/SEC WHICH IS ONLY TRUE IF THE CROSS SECTIONS ARE IN UNITS
 CM**2. IF THE CROSS SECTIONS ARE IN ANY OTHER UNITS (E.G., BARNS)
 ONE SHOULD SIMPLY IGNOR THE IDENTIFICATION CM**3/SEC AND INTERPRET
 THE RESULTS AS BEING IN THE APPROPRIATE UNITS (E.G., FOR CROSS
 SECTION IN BARNS THE REACTION RATE WILL BE IN BARNS*CM/SEC).

 PREPARATION OF CROSS SECTIONS AND WEIGHTING SPECTRUM
 ==================================================================
 PROGRAM LINTAB IS DESIGNED TO CREATE LINEARLY INTERPOLABLE CROSS
 SECTIONS OR WEIGHTING SPECTRUM IN EXACTLY THE FORM WHICH IS USED
 AS INPUT TO THIS PROGRAM.

 METHOD
 ==================================================================
 SPECTRUM AVERAGED REACTION RATES
 ------------------------------------------------------------------
 SPECTRUM AVERAGED REACTION RATES ARE DEFINED AS,

 (INTEGRAL E=0 TO INFINITY) C(KT)*(XC(E)*V(E)*SPECTRUM(E,KT)*DE)

 WHERE,
 E                = ENERGY (SAME UNITS FOR ALL VARIABLES)
 XC(E)            = CROSS SECTION
 SPECTRUM(E,KT)   = ENERGY DEPENDENT SPECTRUM (E.G., MAXWELLIAN)
 V(E)             = SPEED (SQRT(2*E/MASS))
 MASS             = ELECTRON MASS (5.43876D-04 AMU)
 KT               = TEMPERATURE (IN SAME UNITS AS ENERGY)
 C(KT)            = SQRT(8/(PI*MASS*KT))/KT
```

```
DF(I,1) = (DF(I+1,0)-DF(I,0))/(X(I+1)-X(I))
DF(I,2) = (DF(I+1,1)-DF(I,1))/(X(I+1)-X(I))
```


DESCRIPTION OF WEIGHTING SPECTRUM

THE WEIGHTING SPECTRUM V(E)*SPECTRUM(E,KT) MAY BE EITHER,
(1) V*MAXWELLIAN (AN ANALYTICAL FUNCTION), OR,
(2) A GENERAL LINEARLY INTERPOLABLE TABULATED WEIGHTING SPECTRUM.

IN ORDER TO CALCULATE RESULTS TO WITHIN THE SAME ACCURACY THIS PROGRAM WILL RUN MUCH FASTER USING THE V*MAXWELLIAN OPTION AS OPPOSED TO USING THE EQUIVALENT TABULATED FUNCTION. AS SUCH IT IS RECOMMENDED THAT THE V*MAXWELLIAN OPTION BE USED UNLESS THE ACTUAL SPECTRUM DIFFERS SIGNIFICANTLY FROM A MAXWELLIAN.

TABULATED LINEARLY INTERPOLABLE DATA

THE CROSS SECTION AND POSSIBLY V*SPECTRUM ARE EACH ASSUMED TO BE GIVEN IN THE FORM OF A TABLE OF (X,Y) PAIRS WHERE LINEAR INTERPOLATION BETWEEN TABULATED VALUES WILL ACCURATELY REPRESENT THE CROSS SECTION OR V*SPECTRUM TO WITHIN A USER SPECIFIED ACCURACY.

THE DETAILS OF THE METHOD USED TO PRODUCE LINEARLY INTERPOLABLE TABULATED DATA IS DESCRIBED IN THE DOCUMENTATION OF PROGRAM LINTAB AND WILL NOT BE REPEATED HERE.

ACCURACY OF RESULTS

IF WE HAVE A MODEL TO DESCRIBE THE ENERGY DEPENDENCE OF A CROSS SECTION WE CAN USE PROGRAM LINTAB TO PRODUCE A TABLE OF LINEARLY INTERPOLABLE CROSS SECTIONS WHICH ARE EQUAL TO THE RESULTS OF THE MODEL AT THE TABULATED VALUES AND CAN ACCURATELY REPRESENT THE RESULTS OF THE MODEL TO WITHIN A USER SPECIFIED UNCERTAINTY FOR ALL ENERGIES BETWEEN TABULATED VALUES. IN THE FOLLOWING THE MODEL RESULTS WILL BE REFERRED TO AS THE TRUE ENERGY DEPENDENCE OF THE CROSS SECTION (TRUE IN THE SENSE OF REPRESENTING THE RESULTS OF THE MODEL WHICH MAY OR MAY NOT ACCURATELY REPRESENT THE EXACT CROSS SECTIONS).

IF THE TABULATED CROSS SECTIONS ACCURATELY REPRESENT THE TRUE ENERGY DEPENDENCE OF THE CROSS SECTIONS TO WITHIN A USER SPECIFIED ACCURACY AND WE DEFINE,

XC(E)	- THE TRUE ENERGY DEPENDENT CROSS SECTION
APPROXC(E)	- THE ENERGY DEPENDENT CROSS SECTION DEFINED BY THE TABULATED CROSS SECTIONS AND LINEAR INTERPOLATION BETWEEN TABULATED VALUES.
ERROK	- THE ALLOWABLE FRACTIONAL DIFFERENCE BETWEEN THE TRUE CROSS SECTIONS AND THE CROSS SECTION BASED ON LINEAR INTERPOLATION OF TABLES.

WE HAVE THE RELATIONSHIP AT ALL ENERGIES,

XC(E)*(1-ERROK) <= APPROXC(E) <= XC(E)*(1+ERROK)

WHEN WE PERFORM THE INTEGRAL,

(E=0 TO INFINITY) C(KT)*(APPROXC(E)*V(E)*SPECTRUM(E,KT)*DE)

AS LONG AS THE CROSS SECTION IS ZERO OR POSITIVE (AS IT PHYSICALLY MUST BE) WE FIND THAT THE INTEGRAL OF THE TABULATED CROSS SECTION WILL BE BETWEEN (1-ERROK) AND (1+ERROK) TIMES THE INTEGRAL OF THE TRUE CROSS SECTIONS. FOR EXAMPLE, IF THE TABULATED CROSS SECTIONS CAN ACCURATELY APPROXIMATE THE TRUE CROSS SECTION TO WITHIN 0.1 PER-CENT, THE INTEGRAL OF THE TABULATED CROSS SECTIONS WILL BE WITHIN 0.1 PER-CENT OF THE INTEGRAL OF THE TRUE CROSS SECTIONS.

THE USER SUPPLIED FUNCTION MUST BE A DOUBLE PRECISION FUNCTION

IF THE TABULATED CROSS SECTIONS ARE CREATED USING PROGRAM LINTAB THE TABULATED CROSS SECTIONS WILL BE EQUAL TO THE TRUE CROSS SECTIONS AT THE ENERGIES AT WHICH THEY ARE TABULATED AND BETWEEN THESE ENERGIES THE TABULATED CROSS SECTIONS WILL GENERALLY UNDERESTIMATE THE TRUE CROSS SECTION AT SOME ENERGIES AND OVERESTIMATE IT AT OTHER ENERGIES. THIS LEADS TO IMPROVED ACCURACY IN THE INTEGRAL OF THE TABULATED CROSS SECTIONS (DUE TO CROSS CANCELLATION OF THE CONTRIBUTIONS TO THE INTEGRAL FROM ENERGY RANGES WHICH UNDER AND OVERESTIMATE THE TRUE CROSS SECTIONS).

NORMALIZED INTEGRATION UNITS

LINEAR INTERPOLATION BETWEEN TABULATED (X,Y) PAIRS MEANS THAT BETWEEN ANY 2 SUCCESSIVE TABULATED POINTS (X1,Y1) AND (X2,Y2) THE CROSS SECTION OR V*SPECTRUM CAN BE REPRESENTED IN THE FROM,

```
Y(X) = ((X2-X)*Y1+(X-X1)*Y2)/(X2-X1)
```

IT IS POSSIBLE TO EXPRESS THE INTEGRAL OF THIS EXPRESSION BETWEEN X1 AND X2 IN ANALYTICAL FORM. HOWEVER, FOR SMALL X INTERVALS (X2-X1) OR RAPIDLY CHANGING VALUES OF Y THE EXPRESSION FOR THE INTEGRAL BECOMES NUMERICALLY UNSTABLE.

NUMERICAL STABILITY CAN BE ACHIEVED BY INTRODUCING A CHANGE OF VARIABLES TO CONVERT THE INTERVAL (X1,X2) INTO AN INTERVAL (-1,1). DEFINING,

```
AVX     = (X2+X1)/2 - AVERAGE VALUE OF X
CX      = (X2-X1)/2 - 1/2 CHANGE IN X
AVY     = (Y2+Y1)/2 - AVERAGE VALUE OF Y
CY      = (Y2-Y1)/2 - 1/2 CHANGE IN Y
```

BOTH X AND Y CAN BE REPRESENTED IN TERMS OF A VARIABLE Z,

```
X   = CX*Z + AVX , Z = -1 TO 1.
Y   = CY*Z + AVY , Z = -1 TO 1.
DX  = CX*DZ
```

WITH THIS CHANGE OF VARIABLES AN INTEGRAL OF THE FORM,

```
(INTEGRAL X1 TO X2)(Y(X)*DX)
```

IS CONVERTED TO THE FORM,

```
CX*(INTEGRAL -1 TO 1)((CY*Z+AVY)*DZ)
```

DURING INTEGRATION ALL TERMS INVOLVING ODD POWERS OF Z (E.G., CY*Z) WILL MAKE NO CONTRIBUTION TO THE INTEGRAL AND THE INTEGRAL IS SIMPLY,

```
2*CX*AVY = (X2-X1)*(Y2+Y1)/2
```

WHICH CAN BE CALCULATED IN A COMPLETELY STABLE MANNER WITH NO CROSS CANCELLATION OF TERMS OR ROUND-OFF PROBLEMS.

SIMILARLY THE INTEGRAL OF THE PRODUCT OF 2 TABULATED LINEARLY INTERPOLABLE FUNCTIONS,

```
(INTEGRAL X1 TO X2)(Y(X)*S(X)*DX) =

CX*(INTEGRAL -1 TO 1)((CY*Z+AVY)*(CS*Z+AVS)*DZ) =

CX*(INTEGRAL -1 TO 1)((CY*CS*Z*Z+(CY*AVS+CS*AVY)*Z+AVY*AVS)*DZ) =
```

2 1-11 I11 NUMBER OF X RANGES (1 TO 100).

2*CX*(AVY*AVS + CY*CS/3)

NOTE, FOR ANY POSITIVE FUNCTION FROM THEIR DEFINITIONS THE AVERAGE VALUE (AVY OR AVS) IS ALWAYS GREATER THAN OR EQUAL TO 1/2 THE CHANGE (CY OR CS), WHICH MEANS THE DOMINANT CONTRIBUTION TO THE INTEGRAL WILL BE AVY*AVS AND ROUND-OFF PROBLEMS ARE AVOIDED SINCE THE 2 TERMS IN THE ABOVE EXPRESSION CANNOT BE APPROXIMATELY EQUAL AND OF OPPOSITE SIGNS.

THIS APPROACH CAN OBVIOUSLY BE EXTENDED TO DEFINE THE PRODUCT OF ANY NUMBER OF LINEAR INTERPOLABLE FUNCTIONS.

BOTH CROSS SECTION AND SPECTRUM TABULATED

DEPENDENCE OF V*SPECTRUM ON TEMPERATURE

WHEN V*SPECTRUM IS TABULATED IT IS ASSUMED THAT THE TABULATED VALUES ARE GIVEN AS (Z,SZ) WHERE THE RELATIONSHIPS,

```
E    = KT*Z
S(E) = SZ(Z)/KT
DE   = KT*DZ
```

CAN BE USED TO TRANSFORM THE SPECTRUM FROM A FUNCTION OF THE DIMENSIONLESS VARIABLE Z TO DEFINE THE SPECTRUM AT ANY GIVEN TEMPERATURE (KT).

WHEN V*SPECTRUM IS READ IT IS INTEGRATED AND THEN NORMALIZED TO UNITY,

(INTEGRAL 0 TO INFINITY)(SZ(Z)*DZ) = 1

SINCE FOR THE ABOVE CHANGE OF VARIABLES SZ(Z)*DZ = S(E)*DE THIS NORMALIZATION WILL BE MAINTAINED WHEN V*SPECTRUM IS DEFINED AND USED AT ANY GIVEN TEMPERATURE.

DEFINITION OF THE INTEGRAL

ONCE V*SPECTRUM IS TRANSFORMED TO A GIVEN TEMPERATURE THE METHOD DESCRIBED ABOVE CAN BE USED TO IMMEDIATELY DEFINE THE INTEGRAL OF THE PRODUCT OF 2 TABULATED LINEARLY INTERPOLABLE FUNCTIONS IN THE FORM,

C(KT)*(SUM OVER I) DE(I)*(AVXC(I)*AVVS(I)+DXC(I)*DVS(I)/3)

WHERE,

```
I         = ENTENDS OVER ALL E INTERVALS IN WHICH THE CROSS
            SECTION AND V*SPECTRUM ARE BOTH LINEARLY INTERPOLABLE
            (I.E., E INTERVALS ARE DEFINED BY THE UNION OF THE
             E VALUES AT WHICH THE CROSS SECTIONS AND V*SPECTRUM
             ARE TABULATED).
AVXC(I)   = (XC(I+1)+XC(I))/2 - AVERAGE VALUE OF CROSS SECTION.
AVVS(I)   = (VS(I+1)+VS(I))/2 - AVERAGE VALUE OF V*SPECTRUM.
DXC(I)    = (XC(I+1)-XC(I))/2 - 1/2 CHANGE OF CROSS SECTION.
DVS(I)    = (VS(I+1)-VS(I))/2 - 1/2 CHANGE OF V*SPECTRUM.
```

CROSS SECTION IS TABULATED AND SPECTRUM IS MAXWELLIAN

IF THE CROSS SECTION IS TABULATED IN LINEARLY INTERPOLABLE FORM AND THE SPECTRUM IS MAXWELLIAN THE WEIGHTING IS V*MAXWELLIAN,

```
S(E)*DE = C(KT)*E*EXP(-E/KT)*DE
C(KT)       = SQRT(8/(PI*MASS*KT))/KT
MASS        = ELECTRON MASS (5.43876D-04 AMU)
```

```
ION    = 320.0 EV
A      = 0.801
```


THE REQUIRED INTEGRAL IS SIMPLY,

```
(INTEGRAL E=0 TO INFINITY) C(KT)*(E*Y(E)*EXP(-E/KT)*DE)
```

THIS INTEGRAL WILL BE PERFORMED BY INTEGRATING BETWEEN TABULATED VALUES OF THE CROSS SECTION,

```
(SUM OVER I)*(INTEGRAL E(I) TO E(I+1))C(KT)*(E*Y(E)*EXP(-E/KT)*DE)
```

INTRODUCING THE CHANGE OF VARIABLES (DESCRIBED ABOVE),

```
AVE     = (E(I+1)+E(I))/2 - AVERAGE VALUE OF E
DE      = (E(I+1)-E(I))/2 - 1/2 CHANGE IN E
AVY     = (Y(I+1)+Y(I))/2 - AVERAGE VALUE OF Y
DY      = (Y(I+1)-Y(I))/2 - 1/2 CHANGE IN Y
```

BOTH E AND Y CAN BE REPRESENTED IN TERMS OF A VARIABLE Z,

```
E    = DE*Z + AVX , Z = -1 TO 1.
Y    = DY*Z + AVY , Z = -1 TO 1.
DE   = DE*DZ
```

AND WITHIN EACH E INTERVAL THE INTEGRAL REDUCES TO INTEGRATING OVER Z (-1,1) THE EXPRESSION,

```
C(KT)*DE*((DE*Z+AVX)*(DY*Z+AVY)*EXP(-(DE*Z+AVX)/KT))*DZ =

C(KT)*DE*EXP(-AVX/KT)*(DE*DY*Z*Z+(DE*AVY+DY*AVX)*Z+AVX*AVY)*
  EXP(-DE*Z/KT)*DZ) =

G(KT)*(A*Z*Z+B*Z+C)*EXP(-F*Z)*DZ
```

WHERE,

```
G(KT) = C(KT)*DE*EXP(-AVX/KT)
A     = DE*DY
B     = (DE*AVY+DY*AVX)
C     = AVX*AVY
F     = DE/KT
```

WHICH CAN BE EXPRESSED IN ANALTYICAL FORM IN TERMS OF NOTHING MORE COMPLICATED THAN EXPONENTIALS. BY DEFINING THE FUNCTIONS,

```
H(N) = (INTEGRAL -1 TO 1)((Z**N)*EXP(-F*Z)*DZ)
```

THE 3 REQUIRED INTEGRALS ARE,

```
H(0) = (EXP(F)-EXP(-F))/F
H(1) = ((1-F)*EXP(F) - (1+F)*EXP(-F))/(F*F)
H(2) = ((2-2*F+F*F)*EXP(F) - (2+2*F+F*F)*EXP(-F))/(F*F*F)
```

AND THE INTEGRAL IS,

```
G(KT)*(A*H(2) + B*H(1) + C*H(0))
```

ALTHOUGH THE REQUIRED INTEGRALS CAN BE EXPRESSED IN THIS SIMPLE FORM CARE MUST BE USED TO AVOID ROUND-OFF PROBLEMS WHEN THESE FUNCTIONS ARE EVALUATED FOR SMALL VALUES OF F (F = DE/KT). FOR F GREATER THAN 0.1 THE FUNCTIONS ARE DEFINED IN TERMS OF THE ABOVE EXPRESSIONS. FOR SMALLER VALUES OF F THE FUNCTIONS ARE DEFINED IN TERMS OF POWER SERIES EXPANSIONS,

```
H(0) = 2*(1+(F**2)/3!+(F**4)/5!+(F**6)/7!+......
H(1) =-2*F*(1/3+(F**2)/(5*3!)+(F**4)/(7*5!)+(F**6)/(9*7!)+...
H(2) = 2*(1/3+(F**2)/(5*2!)+(F**4)/(7*4!)+(F**6)/(9*6!)+....
```

MESSAGES. THE USER SHOULD CAREFULLY CHECK THIS LISTING AND IF

THESE POWER SERIES EXPANSIONS ARE TRUNCATED AT F**10, WHICH FOR FOR F = 0.1 OR LESS WILL YIELD RESULTS TO AT LEAST 10 DIGITS ACCURACY.

WHEN INTEGRATING LARGER F INTERVALS THE ANALYTICAL EXPRESSIONS FOR H(0), H(1) AND H(2) YIELD NUMERICALLY STABLE RESULTS. IN ORDER TO INVESTIGATE THE NUMERICAL STABILITY IN THE SMALL F LIMIT AS F APPROACHES 0.0 WE CAN START FROM THE INTEGRAL,

G(KT)*(A*Z*Z+B*Z+C)*EXP(-F*Z)*DZ

AND EXPAND THE EXPONENTIAL TO FIRST ORDER IN F TO FIND,

G(KT)*(A*Z*Z+B*Z+C)*(1.-F*Z)*DZ =

G(KT)*(-F*A*Z*Z*Z + (A-B*F)*Z*Z + (B-C*F)*Z + C)*DZ

WHEN WE INTEGRATE OVER Z (-1,1) ALL ODD POWERS OF Z WILL MAKE NO CONTRIBUTION TO THE INTEGRAL AND THE RESULT IS,

G(KT)*2*((A-B*F)/3 + C)

IN THE LIMIT AS F APPROCHES ZERO THIS EXPRESSION APPROACHES THE LIMIT OF THE INTEGRAL OF THE PRODUCT OF 2 LINEARLY INTERPOLABLE FUNCTIONS,

G(KT)*2*(A/3 + C)

IF WE EXAMINE THE ABOVE POWER SERIES WE CAN EASILY SEE THAT THIS IS EXACTLY THE LIMITS OBTAINED. IT IS IMPORATANT TO NOTE THAT THIS LIMIT IS APPROACHED WITHOUT ANY CROSS CANCELLATION OF TERMS WHICH LEADS TO A COMPLETELY NUMERICALLY STABLE ALGORITHM.

TABULATED ENERGY RANGE OF CROSS SECTIONS AND SPECTRUM

WHEN CALCULATING INTEGRALS THIS PROGRAM WILL ASSUME THAT OUTSIDE THE RANGE IN WHICH CROSS SECTIONS OR V*SPECTRUM ARE TABULATED THEY ARE ZERO (I.E., THE PROGRAM DOES NOT HAVE ANY CONVENTIONS OR APPROXIMATIONS HARD WIRED INTO IT TO EXTEND DATA OUTSIDE THE RANGE WHERE IT IS DEFINED). THIS CONVENTION IS USED IN ORDER TO GIVE THE USER MAXIMUM CONTROL OVER HOW DATA IS INTERPRETED AND MINIMIZE THE DECISIONS MADE BY THIS PROGRAM.

WHEN CALCULATING REACTION AVERAGES THE UPPER E LIMIT OF THE INTEGRALS WILL BE TRUNCATED AT,

(1) BOTH TABULATED - THE UPPER E LIMIT OF THE TABULATED CROSS SECTIONS OR V*SPECTRUM, WHICHEVER IS LOWER.

(2) MAXWELLIAN - E = 100*KT OR THE UPPER E LIMIT OF THE TABULATED CROSS SECTIONS, WHICHEVER IS LOWER.

IN PARTICULAR IT IS IMPORTANT TO REALIZE THAT THE PROGRAM WILL NOT ATTEMPT TO EXTEND THE CROSS SECTIONS AS CONSTANT OR IN ANY OTHER FUNCTIONAL FORM ABOVE THE HIGHEST E AT WHICH THEY ARE TABULATED. RATHER THE APPROACH OF TRUNCATING THE INTEGRAL AT THE UPPER ENERGY LIMIT OF THE TABULATED CROSS SECTIONS IS EQUIVALENT TO ASSUMING THAT THE CROSS SECTION IS EQUAL TO 0.0 ABOVE THIS ENERGY LIMIT.

FOR EACH SET OF CROSS SECTIONS THE PROGRAM WILL COMPARE THE HIGHEST TEMPERATURE TO THE HIGHEST ENERGY AT WHICH CROSS SECTIONS ARE TABULATED AND PRINT A WARNING MESSAGE IF THE CROSS SECTIONS ARE NOT TABULATED TO A SUFFIFIENTLY HIGH ENERGY. THE WARNING MESSAGE WILL INFORM THE USER THAT CROSS SECTIONS SHOULD BE TABULATED TO HIGHER ENERGIES AND FAILURE TO DO SO MAY LEAD TO ERRONEOUS RESULTS AT HIGHER TEMPERATURES. AFTER PRINTIONG THE WARNING MESSAGE THE PROGRAM WILL PROCEED WITH THE CALCULATION.

THE INABILITY OF THIS PROGRAM TO DEFINE INTEGRALS WHERE THE CROSS SECTIONS ARE NOT DEFINED SHOULD NOT BE CONSIDERED TO BE A PROBLEM INTRODUCED BY THIS PROGRAM. THE PROBLEM IS THAT IF ONE CANNOT ACCURATELY DESCRIBE THE CROSS SECTIONS AT HIGHER ENERGIES ONE SHOULD NOT EXPECT TO BE ABLE TO ACCURATELY DEFINE THE INTEGRALS. THE WARNING MESSAGE DESCRIBED ABOVE IS INTENDED TO INFORM THE USER THAT IF CROSS SECTIONS CAN BE RELIABLY EXTENDED TO HIGHER ENERGIES THEY SHOULD BE AND THE PROGRAM CAN THEN BE RUN AGAIN. IF THE CROSS SECTIONS CANNOT BE RELIABLY EXTENDED THE TEMPERATURE RANGE SHOULD BE RESTRICTED TO LOWER VALUES.

IN ORDER TO INSURE THAT THE INTEGRALS ARE NOT PREMATURELY TRUNCATED IT IS RECOMMENDED THAT CROSS SECTIONS AND V*SPECTRUM BE TABULATED UP TO ENERGIES CORRESPONDING TO 100 TIMES THE MAXIMUM TEMPERATURE (KT) USED IN THE CALCULATION. FOR MOST CASES THIS IS REALLY 'OVER KILL' IN THE SENSE THAT THE CONTRIBUTION OF VERY HIGH ENERGIES WILL MAKE A NEGLIABLE CONTRIBUTION TO THE INTEGRAL. HOWEVER, IF YOU CAN RELIABLY EXTEND THE CROSS SECTIONS AND V*SPECTRUM TO SUCH HIGH ENERGIES YOU ARE GUARANTEED TO AVOID ALL PROBLEMS INVOLVING TRUNCATING THE UPPER LIMIT OF THE INTEGRAL.

IF A TABULATED V*SPECTRUM IS USED IT SHOULD BE TABULATED BETWEEN 0.0 AND 100.0 (CORRESPONDING TO E/KT = 0.0 TO 100.0).

FOR HIGH TEMPERATURES THE CROSS SECTION MAY HAVE TO BE TABULATED TO VERY HIGH ENERGIES (E.G., IF THE ABOVE RECOMMENDATION IS FOLLOWED, FOR TEMPERATURES UP TO 10 KEV THE CROSS SECTION WOULD HAVE TO BE TABULATED UP TO 1 MEV). IF YOU ARE USING A MODEL WHICH CAN RELIABLY DEFINE THE CROSS SECTIONS TO SUCH HIGH ENERGIES YOU CAN SIMPLY EXTEND THE UPPER ENERGY LIMIT OF THE TABULATED CROSS SECTIONS. IF YOU CANNOT RELIABLY DEFINE THE CROSS SECTION AT SUCH HIGH ENERGIES, BASED EITHER ON A MODEL OR A GOOD GUESS, YOU SHOULD RESTRICT THE RANGE OF TEMPERATURES USED IN CALCULATIONS.

IF YOU WISH TO EXTEND THE CROSS SECTION TO HIGHER ENERGIES AS CONSTANT, YOU NEED ONLY ADD AN ADDITIONAL POINT AT THE END OF THE TABULATED CROSS SECTIONS. THE ADDITIONAL POINT SHOULD SPECIFY THE HIGHEST ENERGY OF INTEREST (E.,G., IN THE EXAMPLE ABOVE 1 MEV) AND THE SAME VALUE OF THE CROSS SECTION AS FOR THE PRECEDING POINT.

IF YOU WISH TO DETERMINE THE EFFECT OF EXTENDING THE CROSS SECTION TO HIGHER ENERGIES YOU CAN RUN THIS PROGRAM SEVERAL TIMES USING DIFFERENT SHAPES FOR THE HIGH ENERGY CROSS SECTIONS (E.G., 0.0, CONSTANT AND RESULTS OF A MODEL) AND COMPARE THE RESULTS. IF THE RESULTS ARE ESSENTIALLY IDENTICAL THIS INDICATES THAT THE RESULTS ARE NOT SENSITIVE TO THE DESCRIPTION OF THE CROSS SECTION AT HIGH ENERGY AND THE RESULTS ARE RELIABLE. ALTERNATIVELY, IF YOU OBTAIN SUFFICIENTLY DIFFERENT RESULTS YOU WILL KNOW THAT THE RESULTS ARE SENSITIVE TO THE DESCRIPTION OF THE HIGH ENERGY CROSS SECTION AND YOU MUST IMPROVE YOUR DESCRIPTION OF THE HIGH ENERGY CROSS SECTION BEFORE YOU CAN USE THIS PROGRAM TO OBTAIN RELIABLE RESULTS.

TEMPERATURE RANGES

THE INPUT PARAMETERS (SEE, DESCRIPTION BELOW) CAN INCLUDE 2 TO 100 TEMPERATURES (KT) WHICH ARE USED TO DEFINE 1 TO 99 TEMPERATURE RANGES. THE PROGRAM WILL TREAT EACH TEMPERATURE RANGE SEPARATELY AND WITHIN EACH RANGE IT WILL TABULATE THE REACTION RATE AT A SUFFICIENT NUMBER OF TEMPERATURES TO ALLOW THE REACTION RATE TO BE ACCURATELY LINEARLY INTERPOLATED TO WITHIN A USER SPECIFIED ACCURACY FOR ALL TEMPERATURES BETWEEN TABULATED VALUES.

THE RUNNING TIME OF THE PROGRAM CAN BE MINIMIZED BY SPECIFYING A NUMBER OF TEMPERATURE RANGES, EACH OF WHICH IS NOT TOO LARGE. IT

IS RECOMMENDED THAT THE USER SPECIFY A NUMBER (4 - 6) OF RANGES PER DECADE OF TEMPERATURE (SEE, EXAMPLE INPUT BELOW).

AVOIDING OVER AND UNDER FLOW

IN PRINCIPLE THE INTEGRALS EXTEND FROM FROM 0.0 TO INFINITY. IN PRACTICE IT IS NOT POSSIBLE TO CALCULATE EXP(E/KT) AS E GOES TO INFINITY. THE STRONGLY CONVERGENT PROPERTIES OF THE MAXWELLIAN ARE USED TO TRUNCATE THE UPPER ENERGY LIMIT OF THE INTEGRAL AT E = 100*KT, WHICH IS WELL BEYOND THE REGION OF INTEREST.

EVEN WITH THIS RESTRICTION ON THE RANGE OF E UNDERFLOW CAN OCCUR WHEN WE DEFINE THE PRODUCT OF SMALL CROSS SECTIONS AND EXP(-F) FOR LARGE F. IN ORDER TO AVOID THIS PROBLEM DURING CALCULATIONS, AFTER THE CROSS SECTIONS ARE READ THE MAXIMUM CROSS SECTION IS DETERMINED AND THE CROSS SECTIONS ARE NORMALIZED BY A FACTOR OF (10**30)/(CROSS SECTION MAXIMUM) (I.E., DURING CALCULATIONS THE CROSS SECTION WILL BE BETWEEN 0.0 AND 10**30). ONCE RESULTS ARE OBTAINED THEY ARE SIMPLY RE-NORMALIZED BY THE RECIPROCAL OF THIS FACTOR TO OBTAIN THE CORRECT RESULTS.

FOR CROSS SECTIONS WHICH HAVE A THRESHOLD, AS THE TEMPERATURE IS DECREASED TOWARD ZERO THE REACTION RATE WILL ALSO APPROACH ZERO. THIS CAN RESULT IN UNDERFLOW AT LOW TEMPERATURES. YOU CAN AVOID THIS PROBLEM BE SPECIFYING A MINIMUM REACTION RATE OF INTEREST, AS DESCRIBED BELOW.

MINIMUM REACTION RATE OF INTEREST

BY USING AN INPUT PARAMETER THE USER CAN CONTROL WHETHER REACTION RATES ARE TABULATED,

(1) BETWEEN THE LOWEST AND HIGHEST SPECIFIED TEMPERATURE, REGARDLESS OF THE MAGNITUDE OF THE REACTION RATE, OR,

(2) BETWEEN THE TEMPERATURE AT WHICH THE REACTION RATE IS EQUAL TO A MINIMUM VALUE (SPECIFIED BY USER INPUT) AND THE HIGHEST SPECIFIED TEMPERATURE.

THE LATER OPTION CAN BE USED TO AVOID UNDERFLOW AT LOW TEMPERATURE AND TO MINIMIZE THE SIZE OF REACTION RATE TABLES BY RESTRICTING THE TABLE TO THE TEMPERATURE RANGE OF PHYSICAL INTEREST (I.E., WHERE THE REACTION RATE IS SIGNIFICANTLY DIFFERENT FROM ZERO).

I/O UNITS

UNIT	DESCRIPTION
5	INPUT PARAMETERS
6	OUTPUT REPORT
10	TABULATED SPECTRUM (IF ANY)
11	TABULATED CROSS SECTIONS
12	TABULATED OUTPUT

INPUT DATA

INPUT DATA IS READ IN THE FOLLOWING ORDER,

(1) INPUT PARAMETERS FROM UNIT 5 (ONLY READ ONCE)

(2) TABULATED WEIGHTING FROM UNIT 10 (ONLY READ IF TABULATED WEIGHTING OPTION IS SELECTED AND THEN ONLY READ ONCE).

(3) TABULATED CROSS SECTIONS FROM UNIT 11 (ONE TABLE AFTER ANOTHER IS READ - NO LIMIT ON THE NUMBER OF TABLES).

ONCE THE INPUT PARAMETERS AND POSSIBLY TABULATED WEIGHTING HAVE BEEN READ, ONE TABLE OF CROSS SECTIONS IS READ AND REACTION RATES ARE CALCULATED AND OUTPUT. THE NEXT TABLE OF CROSS SECTIONS IS THEN READ AND REACTION RATES ARE CALCULATED AND OUTPUT. THE CYCLE

36 3.53076+ 1 8.49211-17 2.84681-18-1.13442-19
37 3.72837+ 1 9.01037-17 2.62263-18-1.03999-19
38 3.94941+ 1 9.53927-17 2.39275-18-1.04074-19

OF READING A TABLE OF CROSS SECTIONS, CALCULATING AND OUTPUTTING IS REPEATED UNTIL ALL TABLES OF CROSS SECTIONS HAVE BEEN PROCESSED (I.E., UNTIL THE END OF FILE IS READ ON UNIT 11).

INPUT PARAMETER FORMAT (UNIT 5)

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-11	I11	WEIGHTING MODEL NUMBER, = 0 - V*MAXWELLIAN = 1 - TABULATED
	12-22	D11.4	MINIMUM REACTION RATE OF INTEREST = 0.0 - NO LOWER LIMIT = OTHERWISE - ONLY TABULATE REACTION RATES AT TEMPERATURES WHERE THEY ARE EQUAL TO OR GREATER THAN THE SPECIFIED MINIMUM.
2-N	1-11	D11.4	TEMPERATURE (KT)
	12-22	D11.4	ALLOWABLE FRACTIONAL UNCERTAINTY

INPUT LINE 2 MAY BE REPEATED UP TO 100 TIMES TO SPECIFY UP TO 99 TEMPERATURE RANGES. TEMPERATURES MUST BE POSITIVE (ZERO IS NOT ALLOWED) AND IN ASCENDING ORDER. ANY TEMPERATURE WHICH IS NOT POSITIVE OR NOT IN ASCENDING ORDER WILL BE IGNORED.

INPUT IS TERMINATED BY THE END OF DATA (I.E., END OF FILE ON UNIT 5).

EXAMPLE INPUT NO. 1

USE A MAXWELLIAN SPECTRUM TO CALCULATE REACTIONS RATES FOR TEMPERATURES BETWEEN 1 EV AND 10 KEV. ONLY TABULATE REACTION RATES AT TEMPERATURES WHERE THE REACTION RATES IS 1.0D-16 OR GREATER. TABULATE REACTION RATES TO WITHIN AN ACCURACY OF 0.1 PER-CENT (INPUT AS A FRACTION 0.001). THE FOLLOWING 3 INPUT CARDS ARE REQUIRED,

```
          0 1.0000D-16
 1.0000D+00 1.0000D-03
 1.0000D+04 1.0000D-03
```

EXAMPLE INPUT NO. 2

PERFORM THE SAME CALCULATION AS ABOVE, BUT SPECIFY 4 TEMPERATURES PER TEMPERATURE DECADE. THIS IS THE RECOMMENDED PROCEDURE AND THIS INPUT WILL MAKE THE PROGRAM RUN FASTER THAN THE ABOVE INPUT. THE FOLLOWING 18 INPUT CARDS ARE REQUIRED,

```
          0 1.0000D-16
 1.0000D+00 1.0000D-03
 2.0000D+00 1.0000D-03
 4.0000D+00 1.0000D-03
 7.0000D+00 1.0000D-03
 1.0000D+01 1.0000D-03
 2.0000D+01 1.0000D-03
 4.0000D+01 1.0000D-03
 7.0000D+01 1.0000D-03
 1.0000D+02 1.0000D-03
 2.0000D+02 1.0000D-03
 4.0000D+02 1.0000D-03
 7.0000D+02 1.0000D-03
 1.0000D+03 1.0000D-03
 2.0000D+03 1.0000D-03
 4.0000D+03 1.0000D-03
 7.0000D+03 1.0000D-03
 1.0000D+04 1.0000D-03
```

101 7.65199+ 3 1.13437-17-1.23561-21 2.67916-25
102 8.08026+ 3 1.08637-17-1.12087-21 2.17739-25

TABULATED DATA

THE FORMAT OF TABULATED DATA (WEIGHTING SPECTRUM, CROSS SECTIONS AND CALCULATED REACTION RATES) ARE ALL IDENTICAL AND ARE DESIGNED TO ALLOW ANY OF THIS DATA TO BE PLOTTED USING PROGRAM PLOTTAB.

TABULATED SPECTRUM FORMAT (UNIT 10)

IF A TABULATED WEIGHTING SPECTRUM IS USED IT MUST BE IN THE FOLLOWING FORMAT. IF USED THIS DATA WILL ONLY BE READ ONCE.

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-72	18A4	PHYSICAL DESCRIPTION OF SPECTRUM
2-N	1-11	D11.4	X
	12-22	D11.4	Y

THE TABLE IS TERMINATED BY A BLANK (NOT 0.0) LINE.

THE TABULATED WEIGHTING SPECTRUM MAY BE REPRESENTED BY UP TO 2000 (X,Y) PAIRS. IF THIS LIMIT IS EXCEEDED ONLY THE FIRST 2000 PAIRS WILL BE USED IN THE CALCULATION. A TABULATED SPECTRUM COULD LOOK LIKE,

```
TABULATED V*MAXWELLIAN (TO WITHIN 0.1 PER-CENT)
 0.00000+ 0 0.00000+ 0
 1.25000- 3 1.24844- 3
 3.43750- 3 3.42570- 3
      .          .
      .          .
      .          .
      .          .
 9.95000+ 1 6.10269-42
 9.97500+ 1 4.76472-42
 1.00000+ 2 3.72007-42
                          (BLANK LINE TERMINATES CURVE)
```

TABULATED CROSS SECTION FORMAT (UNIT 11)

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-72	18A4	PHYSICAL DESCRIPTION OF CROSS SECTIONS
2-N	1-11	D11.4	X
	12-22	D11.4	Y

A TABLE IS TERMINATED BY A BLANK (NOT 0.0) LINE.

THIS FILE MAY CONTAIN ANY NUMBER OF CROSS SECTION TABLES. CROSS SECTION TABLES WILL BE PROCESSED ONE AFTER ANOTHER UNTIL ALL TABLES HAVE BEEN PROCESSD (I.E., UNTIL AN END OF FILE IS READ).

EACH TABLE OF CROSS SECTIONS MAY BE REPRESENTED BY UP TO 2000 (X,Y) PAIRS. IF THIS LIMIT IS EXCEEDED ONLY THE FIRST 2000 PAIRS WILL BE USED IN THE CALCULATION AND THIS WILL BE TREATED AS AN END OF FILE ON UNIT 11 (I.E., THE PROGRAM DOES NOT KNOW WHERE THE BEGINNING OF THE NEXT TABLE IS).

A SERIES OF CROSS SECTION TABLES COULD LOOK LIKE,

```
O I
 1.36000+ 1 0.00000+ 0
 1.36053+ 1 5.76581-20
 1.36159+ 1 1.72538-19
      .          .
```

I/O UNIT 4 CONTAINS CONTROL INFORMATION OF TWO TYPES

```
165 2.76082+ 5
166 2.91534+ 5 5.22908-19-1.66361-24 9.55361-30
167 3.08818+ 5 4.97008-19-1.49849-24 8.60908-30
```



```
     .           .
 9.83251+ 5 1.77360-19
 1.00000+ 6 1.74694-19
                          (BLANK LINE TERMINATES CURVE)
O II
 3.51000+ 1 0.00000+ 0
 3.51274+ 1 5.90426-20
 3.51822+ 1 1.76683-19
     .           .
     .           .
 9.82549+ 5 5.01209-20
 1.00000+ 6 4.93228-20
                          (BLANK LINE TERMINATES CURVE)
O III
 5.49000+ 1 0.00000+ 0
 5.49428+ 1 3.89652-20
 5.50286+ 1 1.16833-19
     .           .
     .           .
 9.90728+ 5 3.26001-22
 1.00000+ 6 3.23406-22
                          (BLANK LINE TERMINATES CURVE)
```

TABULATED REACTION RATE FORMAT (UNIT 12)

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-72	18A4	PHYSICAL DESCRIPTION OF CROSS SECTIONS (COPIED FROM TABULATED CROSS SECTION FILE).
2-N	1-11	D11.4	X
	12-22	D11.4	Y

A TABLE IS TERMINATED BY A BLANK (NOT 0.0) LINE.

FOR EACH CROSS SECTION TABLE READ REACTION RATES ARE CALCULATED AND OUTPUT. CALCULATIONS CONTINUE UNTIL ALL CROSS SECTION TABLES HAVE BEEN READ (I.E., END OF FILE ON UNIT 11).

THE REACTION RATE OUTPUT CORRESPONDING TO EXAMPLE INPUT NO. 2 AND THE ABOVE CROSS SECTIONS COULD LOOK LIKE (NOTE, FOR O I REACTION RATES ARE TABULATED FROM 1 EV TO 10 KEV, WHEREAS O II AND O III ARE TABULATED FROM THE LOWEST TEMPERATURE WHERE THE REACTION RATE IS EQUAL TO 1.0-16 UP TO A TEMPERATURE OF 10 KEV),

```
O I
 1.00000+ 0 9.92784-15
 1.00625+ 0 1.08282-14
 1.01250+ 0 1.17976-14
     .           .
     .           .
 9.85000+ 3 5.48140- 8
 1.00000+ 4 5.45808- 8
                          (BLANK LINE TERMINATES CURVE)
O II
 1.94840+ 0 1.00000-16
 1.95753+ 0 1.08988-16
 1.96531+ 0 1.17215-16
     .           .
     .           .
 9.85000+ 3 1.77737- 8
 1.00000+ 4 1.76868- 8
                          (BLANK LINE TERMINATES CURVE)
O III
 3.07849+ 0 1.00000-16
 3.08750+ 0 1.05425-16
```

```
15 3.84089+ 1 6.17378-18 1.64299-18-1.33419-19
16 3.88914+ 1 6.93547-18 1.57862-18-1.19575-19
```



```
 3.10000+ 0 1.13463-16
      .          .
      .          .
 9.85000+ 3 8.76818- 9
 1.00000+ 4 8.72463- 9
                           (BLANK LINE TERMINATES CURVE)
```

OUTPUT REACTION RATES
===

THE PROGRAM WILL OUTPUT THE (X,Y) PAIRS DESCRIBING THE FUNCTION ON UNIT 12 (AS DESCRIBED ABOVE). IN ADDITION THE PROGRAM WILL OUTPUT ON UNIT 6 A LISTING PRESENTING NOT ONLY THE X VALUE AND THE VALUE OF THE FUNCTION (Y), BUT ALSO THE LOCAL APPROXIMATION TO THE FIRST AND SECOND DERIVATIVES (DESCRIBED ABOVE) AND WARNING AND/OR ERROR MESSAGES. THE USER SHOULD CAREFULLY CHECK THIS LISTING AND IF NECESSARY TAKE CORRECTIVE ACTION BEFORE USING THE TABULATED DATA IN ANY APPLICATION.

===

Example HEATER output

The following page illustrates the results obtained using program HEATER for the example problem distributed with this program. The plot was produced using program PLOTTAB.

CALCULATE SPECTRUM AVERAGED REACTION RATES (HEATER 87-1)

DESCRIPTION OF SPECTRUM............ MAXWELLIAN
MINIMUM REACTION RATE OF INTEREST... 1.00000-16 CM**3/SEC

TEMPERATURE RANGES

INDEX	TEMPERATURE (EV)	ALLOWABLE FRACTIONAL UNCERTAINTY	
1	1.00000+ 0	1.00000- 3	(0.10000 PER-CENT)
2	2.00000+ 0	1.00000- 3	(0.10000 PER-CENT)
3	4.00000+ 0	1.00000- 3	(0.10000 PER-CENT)
4	7.00000+ 0	1.00000- 3	(0.10000 PER-CENT)
5	1.00000+ 1	1.00000- 3	(0.10000 PER-CENT)
6	2.00000+ 1	1.00000- 3	(0.10000 PER-CENT)
7	4.00000+ 1	1.00000- 3	(0.10000 PER-CENT)
8	7.00000+ 1	1.00000- 3	(0.10000 PER-CENT)
9	1.00000+ 2	1.00000- 3	(0.10000 PER-CENT)
10	2.00000+ 2	1.00000- 3	(0.10000 PER-CENT)
11	4.00000+ 2	1.00000- 3	(0.10000 PER-CENT)
12	7.00000+ 2	1.00000- 3	(0.10000 PER-CENT)
13	1.00000+ 3	1.00000- 3	(0.10000 PER-CENT)
14	2.00000+ 3	1.00000- 3	(0.10000 PER-CENT)
15	4.00000+ 3	1.00000- 3	(0.10000 PER-CENT)
16	7.00000+ 3	1.00000- 3	(0.10000 PER-CENT)
17	1.00000+ 4	0.00000+ 0	(0.00000 PER-CENT)

SUMMARY OF CROSS SECTIONS

TITLE

O I -> II (q = 0) Belfast Recommendation

E-MINIMUM (EV)	E-MAXIMUM (EV)	POINTS
1.36000+ 1	1.00000+ 6	188

TABULATED RESULTS

POINT	TEMPERATURE (EV)	REACTION RATE (CM**3/SEC)	FIRST DERIVATIVE	SECOND DERIVATIVE	
1	1.00000+ 0	9.92797-15			END OF RANGE
2	1.00625+ 0	1.08283-14	1.44051-13	1.77070-12	
3	1.01250+ 0	1.17978-14	1.55118-13	1.88082-12	
4	1.01875+ 0	1.28407-14	1.66873-13	1.99603-12	
5	1.02500+ 0	1.39616-14	1.79348-13	2.11646-12	
6	1.03125+ 0	1.51653-14	1.92576-13	2.24225-12	
7	1.03750+ 0	1.64564-14	2.06590-13	2.37353-12	
8	1.04375+ 0	1.78403-14	2.21425-13	2.51044-12	
9	1.05000+ 0	1.93223-14	2.37115-13	2.65312-12	
10	1.05625+ 0	2.09079-14	2.53697-13	2.80170-12	
11	1.06250+ 0	2.26030-14	2.71208-13	2.95631-12	
12	1.06875+ 0	2.44135-14	2.89685-13	3.11709-12	
13	1.07500+ 0	2.63458-14	3.09166-13	3.28417-12	
14	1.08125+ 0	2.84064-14	3.29693-13	3.45767-12	
15	1.08750+ 0	3.06020-14	3.51303-13	3.63773-12	
16	1.09375+ 0	3.29397-14	3.74039-13	3.82447-12	

MASS = ELECTRON MASS (5.43876D-04 AMU)
KT = TEMPERATURE (IN SAME UNITS AS ENERGY)
C(KT) = SQRT(8/(PI*MASS*KT))/KT

17	1.10000+ 0	3.54269-14	3.97942-13	4.01801-12
18	1.10625+ 0	3.80710-14	4.23054-13	4.21848-12
19	1.11250+ 0	4.08799-14	4.49420-13	4.42599-12
20	1.11875+ 0	4.38616-14	4.77082-13	4.64067-12
21	1.12500+ 0	4.70247-14	5.06087-13	4.86263-12
22	1.13125+ 0	5.03776-14	5.36478-13	4.27695-12
23	1.14062+ 0	5.57800-14	5.76553-13	5.44796-12
24	1.15000+ 0	6.16674-14	6.27655-13	5.82931-12
25	1.15937+ 0	6.80603-14	6.82276-13	6.21596-12
26	1.16875+ 0	7.50069-14	7.40582-13	6.63367-12
27	1.17812+ 0	8.25286-14	8.02739-13	7.05564-12
28	1.18750+ 0	9.06791-14	8.68921-13	7.51108-12
29	1.19687+ 0	9.94803-14	9.39300-13	7.96951-12
30	1.20625+ 0	1.08992-13	1.01405-12	8.46392-12
31	1.21562+ 0	1.19237-13	1.09336-12	8.95982-12
32	1.22500+ 0	1.30281-13	1.17740-12	9.49429-12
33	1.23437+ 0	1.42147-13	1.26636-12	1.00285-11
34	1.24375+ 0	1.54908-13	1.36043-12	1.06040-11
35	1.25312+ 0	1.68586-13	1.45979-12	1.11774-11
36	1.26250+ 0	1.83262-13	1.56464-12	1.17947-11
37	1.27187+ 0	1.98958-13	1.67515-12	1.24077-11
38	1.28125+ 0	2.15763-13	1.79154-12	1.30676-11
39	1.29062+ 0	2.33697-13	1.91398-12	1.37207-11
40	1.30000+ 0	2.52857-13	2.04268-12	1.44237-11
41	1.30937+ 0	2.73264-13	2.17783-12	1.51172-11
42	1.31875+ 0	2.95022-13	2.31963-12	1.58636-11
43	1.32812+ 0	3.18150-13	2.46827-12	1.65976-11
44	1.33750+ 0	3.42762-13	2.62396-12	1.52867-11
45	1.35000+ 0	3.77950-13	2.81504-12	1.84427-11
46	1.36250+ 0	4.16020-13	3.04557-12	1.95425-11
47	1.37500+ 0	4.57143-13	3.28986-12	2.06798-11
48	1.38750+ 0	5.01498-13	3.54835-12	2.18542-11
49	1.40000+ 0	5.49267-13	3.82153-12	2.30656-11
50	1.41250+ 0	6.00640-13	4.10985-12	2.43138-11
51	1.42500+ 0	6.55812-13	4.41377-12	2.55984-11
52	1.43750+ 0	7.14984-13	4.73375-12	2.69191-11
53	1.45000+ 0	7.78362-13	5.07024-12	2.82755-11
54	1.46250+ 0	8.46158-13	5.42368-12	2.96672-11
55	1.47500+ 0	9.18590-13	5.79452-12	3.10936-11
56	1.48750+ 0	9.95880-13	6.18319-12	3.25543-11
57	1.50000+ 0	1.07825-12	6.59012-12	3.40488-11
58	1.51250+ 0	1.16595-12	7.01573-12	3.55763-11
59	1.52500+ 0	1.25921-12	7.46043-12	3.71363-11
60	1.53750+ 0	1.35826-12	7.92464-12	3.87281-11
61	1.55000+ 0	1.46337-12	8.40874-12	4.03511-11
62	1.56250+ 0	1.57479-12	8.91313-12	4.20044-11
63	1.57500+ 0	1.69277-12	9.43818-12	3.66434-11
64	1.59375+ 0	1.88261-12	1.01252-11	4.62686-11
65	1.61250+ 0	2.08873-12	1.09928-11	4.89090-11
66	1.63125+ 0	2.31204-12	1.19098-11	5.16089-11
67	1.65000+ 0	2.55349-12	1.28775-11	5.43652-11
68	1.66875+ 0	2.81406-12	1.38968-11	5.71751-11
69	1.68750+ 0	3.09472-12	1.49689-11	6.00355-11
70	1.70625+ 0	3.39650-12	1.60945-11	6.29432-11
71	1.72500+ 0	3.72040-12	1.72747-11	6.58953-11
72	1.74375+ 0	4.06746-12	1.85103-11	6.88885-11
73	1.76250+ 0	4.43875-12	1.98019-11	7.19198-11
74	1.78125+ 0	4.83532-12	2.11504-11	7.49858-11
75	1.80000+ 0	5.25825-12	2.25564-11	7.89122-11
76	1.81835+ 0	5.69873-12	2.40044-11	7.35881-11
77	1.84105+ 0	6.28155-12	2.56749-11	9.08648-11
78	1.86091+ 0	6.82730-12	2.74795-11	7.95367-11
79	1.88589+ 0	7.56336-12	2.94663-11	1.01322-10
80	1.90681+ 0	8.22414-12	3.15860-11	9.14179-11
81	1.93010+ 0	9.00937-12	3.37151-11	1.16496-10

CAN ACCURATELY APPROXIMATE THE TRUE CROSS SECTION TO WITHIN 0.1 PER-CENT, THE INTEGRAL OF THE TABULATED CROSS SECTIONS WILL BE WITHIN 0.1 PER-CENT OF THE INTEGRAL OF THE TRUE CROSS SECTIONS.

82	1.94757+ 0	9.63392-12	3.57503-11	8.64268-11	
83	1.97378+ 0	1.06303-11	3.80155-11	1.60455-10	
84	1.98689+ 0	1.11563-11	4.01191-11	1.10025-10	
85	2.00000+ 0	1.17011-11			END OF RANGE
86	2.02500+ 0	1.27940-11	4.37144-11	1.16623-10	
87	2.05000+ 0	1.39598-11	4.66300-11	1.20940-10	
88	2.07500+ 0	1.52011-11	4.96535-11	1.25242-10	
89	2.10000+ 0	1.65207-11	5.27845-11	1.29524-10	
90	2.12500+ 0	1.79213-11	5.60226-11	1.33779-10	
91	2.15000+ 0	1.94054-11	5.93671-11	1.38004-10	
92	2.17500+ 0	2.09759-11	6.28172-11	1.42194-10	
93	2.20000+ 0	2.26352-11	6.63721-11	1.22525-10	
94	2.23750+ 0	2.52964-11	7.09667-11	1.52482-10	
95	2.27500+ 0	2.81721-11	7.66848-11	1.58513-10	
96	2.31250+ 0	3.12707-11	8.26290-11	1.64423-10	
97	2.35000+ 0	3.46005-11	8.87949-11	1.70200-10	
98	2.38750+ 0	3.81697-11	9.51774-11	1.75837-10	
99	2.42500+ 0	4.19861-11	1.01771-10	1.81325-10	
100	2.46250+ 0	4.60575-11	1.08571-10	1.86657-10	
101	2.50000+ 0	5.03914-11	1.15571-10	1.91829-10	
102	2.53750+ 0	5.49951-11	1.22764-10	1.96834-10	
103	2.57500+ 0	5.98755-11	1.30145-10	2.51432-10	
104	2.60000+ 0	6.32863-11	1.36431-10	1.54368-10	
105	2.65000+ 0	7.04938-11	1.44150-10	2.10811-10	
106	2.70000+ 0	7.82283-11	1.54690-10	2.16521-10	
107	2.75000+ 0	8.65041-11	1.65516-10	2.21916-10	
108	2.80000+ 0	9.53347-11	1.76612-10	2.26995-10	
109	2.85000+ 0	1.04733-10	1.87962-10	2.31760-10	
110	2.90000+ 0	1.14710-10	1.99550-10	2.36215-10	
111	2.95000+ 0	1.25278-10	2.11361-10	2.40363-10	
112	3.00000+ 0	1.36447-10	2.23379-10	2.44209-10	
113	3.05000+ 0	1.48227-10	2.35589-10	2.47760-10	
114	3.10000+ 0	1.60626-10	2.47977-10	2.09604-10	
115	3.17500+ 0	1.80403-10	2.63697-10	2.55364-10	
116	3.25000+ 0	2.01617-10	2.82850-10	2.59128-10	
117	3.32500+ 0	2.24288-10	3.02284-10	2.62316-10	
118	3.40000+ 0	2.48435-10	3.21958-10	2.64957-10	
119	3.47500+ 0	2.74072-10	3.41830-10	2.67081-10	
120	3.55000+ 0	3.01212-10	3.61861-10	3.35713-10	
121	3.60000+ 0	3.20144-10	3.78647-10	2.02341-10	
122	3.70000+ 0	3.60032-10	3.98881-10	2.66538-10	
123	3.80312+ 0	4.03999-10	4.26366-10	2.59713-10	
124	3.91562+ 0	4.55252-10	4.55584-10	4.96489-10	
125	3.95781+ 0	4.75357-10	4.76531-10	2.70387-10	
126	4.00000+ 0	4.95943-10			END OF RANGE
127	4.11250+ 0	5.53183-10	5.08796-10	2.68360-10	
128	4.22500+ 0	6.13819-10	5.38987-10	2.66215-10	
129	4.33750+ 0	6.77824-10	5.68936-10	2.63555-10	
130	4.45000+ 0	7.45165-10	5.98586-10	2.27557-10	
131	4.60000+ 0	8.40073-10	6.32719-10	2.55686-10	
132	4.75000+ 0	9.40734-10	6.71072-10	2.50381-10	
133	4.90000+ 0	1.04703- 9	7.08629-10	2.44619-10	
134	5.05000+ 0	1.15883- 9	7.45322-10	2.38495-10	
135	5.20000+ 0	1.27599- 9	7.81097-10	1.92494-10	
136	5.42500+ 0	1.46148- 9	8.24408-10	2.22102-10	
137	5.65000+ 0	1.65822- 9	8.74381-10	2.11863-10	
138	5.87500+ 0	1.86568- 9	9.22050-10	2.53327-10	
139	6.02500+ 0	2.00969- 9	9.60049-10	1.44234-10	
140	6.32500+ 0	2.31068- 9	1.00332- 9	1.80941-10	
141	6.62500+ 0	2.62796- 9	1.05760- 9	2.19987-10	
142	6.81250+ 0	2.83400- 9	1.09885- 9	1.59431-10	
143	7.00000+ 0	3.04564- 9			END OF RANGE
144	7.30000+ 0	3.39522- 9	1.16529- 9	1.14429-10	
145	7.75000+ 0	3.94278- 9	1.21678- 9	1.22064-10	
146	8.20000+ 0	4.51505- 9	1.27171- 9	9.14610-11	

CX*(INTEGRAL -1 TO 1)((CY*Z+AVY)*(CS*Z+AVS)*DZ) =

CX*(INTEGRAL -1 TO 1)((CY*CS*Z*Z+(CY*AVS+CS*AVY)*Z+AVY*AVS)*DZ) =

147	8.80000+ 0	5.31100- 9	1.32659- 9	7.71634-11	
148	9.55000+ 0	6.34935- 9	1.38446- 9	2.14913-10	
149	9.70000+ 0	6.56185- 9	1.41670- 9	6.26409-11	
150	9.85000+ 0	6.77577- 9	1.42610- 9	5.90422-11	
151	1.00000+ 1	6.99101- 9			END OF RANGE
152	1.10000+ 1	8.45441- 9	1.46340- 9	2.27189-11	
153	1.30000+ 1	1.14721- 8	1.50884- 9	2.59820-12	
					WARNING-INFLECTION POINT
154	1.65000+ 1	1.67848- 8	1.51793- 9	-1.89035-11	
155	1.90000+ 1	2.04615- 8	1.47067- 9	-7.27668-11	
156	1.95000+ 1	2.11787- 8	1.43429- 9	-2.68412-11	
157	2.00000+ 1	2.18891- 8			END OF RANGE
158	2.20000+ 1	2.46604- 8	1.38563- 9	-2.93917-11	
159	2.40000+ 1	2.73141- 8	1.32684- 9	-2.99473-11	
160	2.60000+ 1	2.98480- 8	1.26695- 9	-2.45954-11	
161	2.90000+ 1	3.34274- 8	1.19316- 9	-2.82660-11	
162	3.20000+ 1	3.67525- 8	1.10837- 9	-2.64122-11	
163	3.50000+ 1	3.98399- 8	1.02913- 9	-2.43875-11	
164	3.80000+ 1	4.27078- 8	9.55966-10	-4.56218-11	
165	3.90000+ 1	4.36182- 8	9.10345-10	-2.17134-11	
166	4.00000+ 1	4.45068- 8			END OF RANGE
167	4.45000+ 1	4.82537- 8	8.32646-10	-1.84222-11	
168	4.90000+ 1	5.16276- 8	7.49747-10	-1.60841-11	
169	5.35000+ 1	5.46757- 8	6.77368-10	-1.40727-11	
170	5.80000+ 1	5.74389- 8	6.14041-10	-1.06621-11	
171	6.40000+ 1	6.07393- 8	5.50068-10	-2.71993-11	
172	6.55000+ 1	6.15032- 8	5.09269-10	-1.00103-11	
173	6.70000+ 1	6.22446- 8	4.94254-10	-9.61361-12	
174	6.85000+ 1	6.29644- 8	4.79834-10	-9.23668-12	
175	7.00000+ 1	6.36633- 8			END OF RANGE
176	7.75000+ 1	6.68733- 8	4.27997-10	-6.66677-12	
177	8.65000+ 1	7.01853- 8	3.67996-10	-5.44923-12	
178	9.70000+ 1	7.34485- 8	3.10779-10	-1.99668-11	
179	9.85000+ 1	7.38697- 8	2.80829-10	-4.51551-12	
180	1.00000+ 2	7.42808- 8			END OF RANGE
181	1.10000+ 2	7.67841- 8	2.50327-10	-3.57403-12	
182	1.20000+ 2	7.89299- 8	2.14586-10	-2.38184-12	
183	1.35000+ 2	8.16128- 8	1.78859-10	-2.25198-12	
184	1.50000+ 2	8.37890- 8	1.45079-10	-1.49461-12	
185	1.70000+ 2	8.60927- 8	1.15187-10	-1.13588-12	
186	1.95000+ 2	8.82625- 8	8.67896-11	-2.97157-12	
187	2.00000+ 2	8.86221- 8			END OF RANGE
188	2.30000+ 2	9.03805- 8	5.86134-11	-5.87229-13	
189	2.60000+ 2	9.16104- 8	4.09965-11	-3.52635-13	
190	3.00000+ 2	9.26861- 8	2.68911-11	-2.17139-13	
191	3.60000+ 2	9.35178- 8	1.38628-11	-6.37384-13	
192	3.70000+ 2	9.35927- 8	7.48895-12	-1.41881-13	
193	3.80000+ 2	9.36534- 8	6.07014-12	-1.30087-13	
194	3.90000+ 2	9.37011- 8	4.76927-12	-1.19421-13	
195	4.00000+ 2	9.37369- 8			END OF RANGE
196	4.90000+ 2	9.36553- 8	-9.06233-13	-3.94071-14	
197	6.40000+ 2	9.26327- 8	-6.81729-12	-1.37503-13	
198	6.55000+ 2	9.24995- 8	-8.87983-12	-1.50871-14	
199	5.70000+ 2	9.23629- 8	-9.10614-12	-1.33758-14	
200	6.85000+ 2	9.22233- 8	-9.30678-12	-1.18293-14	
201	7.00000+ 2	9.20811- 8			END OF RANGE
202	7.15000+ 2	9.19364- 8	-9.64067-12	-9.16270-15	
203	7.30000+ 2	9.17898- 8	-9.77811-12	-8.01348-15	
204	7.45000+ 2	9.16413- 8	-9.89831-12	-6.97038-15	
205	7.60000+ 2	9.14913- 8	-1.00029-11	-6.02274-15	
206	7.75000+ 2	9.13399- 8	-1.00932-11	-5.16112-15	
207	7.90000+ 2	9.11873- 8	-1.01706-11	-4.37710-15	
208	8.05000+ 2	9.10338- 8	-1.02363-11	-3.66322-15	
209	8.20000+ 2	9.08794- 8	-1.02912-11	-3.01280-15	
210	8.35000+ 2	9.07243- 8	-1.03364-11	-2.41988-15	

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S(E)*DE = C(KT)*E*EXP(-E/KT)*DE
C(KT)       = SQRT(8/(PI*MASS*KT))/KT
MASS        = ELECTRON MASS (5.43876D-04 AMU)
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211	8.50000+ 2	9.05688- 8	-1.03727-11	-1.87913-15	
212	8.65000+ 2	9.04127- 8	-1.04009-11	-1.38576-15	
213	8.80000+ 2	9.02564- 8	-1.04217-11	-9.35474-16	
214	8.95000+ 2	9.00999- 8	-1.04357-11	-5.24419-16	
215	9.10000+ 2	8.99432- 8	-1.04436-11	-1.49112-16	
					WARNING-INFLECTION POINT
216	9.25000+ 2	8.97865- 8	-1.04458-11	1.93583-16	
217	9.40000+ 2	8.96299- 8	-1.04429-11	5.06501-16	
218	9.55000+ 2	8.94734- 8	-1.04353-11	7.92201-16	
219	9.70000+ 2	8.93170- 8	-1.04234-11	1.05300-15	
220	9.85000+ 2	8.91609- 8	-1.04076-11	1.29101-15	
221	1.00000+ 3	8.90051- 8			END OF RANGE
222	1.45000+ 3	8.46034- 8	-9.78157-12	3.21157-15	
223	1.90000+ 3	8.08520- 8	-8.33637-12	1.51339-14	
224	1.95000+ 3	8.04730- 8	-7.57967-12	2.76887-15	
225	2.00000+ 3	8.01009- 8			END OF RANGE
226	2.50000+ 3	7.67226- 8	-6.75663-12	2.06193-15	
227	3.00000+ 3	7.38598- 8	-5.72567-12	1.42617-15	
228	3.60000+ 3	7.09378- 8	-4.86997-12	4.44994-15	
229	3.70000+ 3	7.04953- 8	-4.42497-12	1.11941-15	
230	3.80000+ 3	7.00640- 8	-4.31303-12	1.07024-15	
231	3.90000+ 3	6.96434- 8	-4.20601-12	1.02404-15	
232	4.00000+ 3	6.92330- 8			END OF RANGE
233	4.75000+ 3	6.64418- 8	-3.72170-12	6.59266-16	
234	5.65000+ 3	6.36262- 8	-3.12836-12	4.87560-16	
235	6.70000+ 3	6.06790- 8	-2.61642-12	1.67541-15	
236	6.85000+ 3	6.05242- 8	-2.36511-12	3.66131-16	
237	7.00000+ 3	6.01777- 8			END OF RANGE
238	8.20000+ 3	5.76654- 8	-2.09360-12	2.43333-16	
239	9.55000+ 3	5.52825- 8	-1.76510-12	1.04139-15	
240	9.70000+ 3	5.50412- 8	-1.60889-12	1.84575-16	
241	9.85000+ 3	5.48040- 8	-1.58121-12	1.78966-16	
242	1.00000+ 4	5.45708- 8			END OF RANGE

SUMMARY OF CROSS SECTIONS

TITLE

O II -> III (q = 1) Belfast Recommendation

E-MINIMUM (EV)	E-MAXIMUM (EV)	POINTS
3.51000+ 1	1.00000+ 6	189

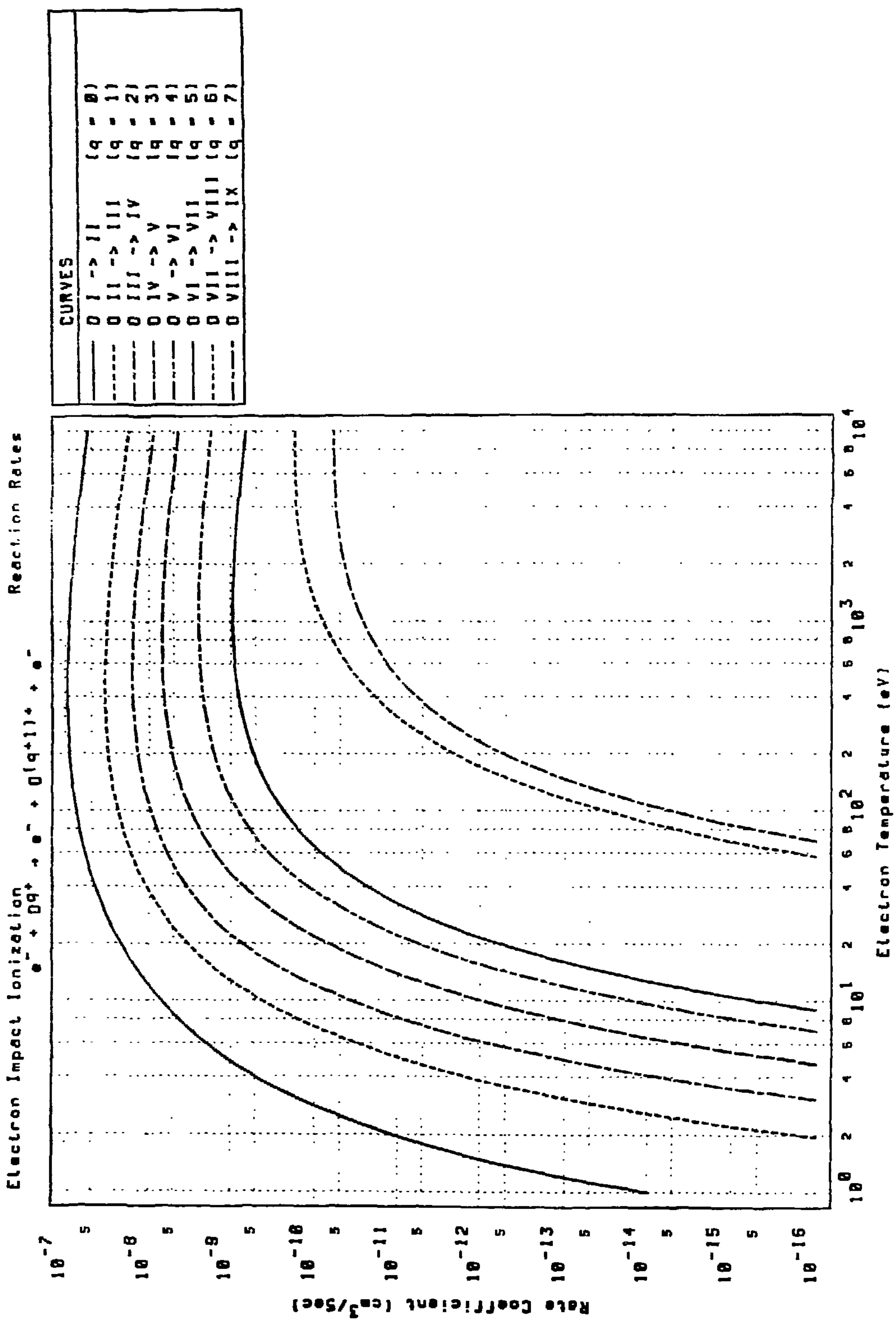
TABULATED RESULTS

POINT	TEMPERATURE (EV)	REACTION RATE (CM**3/SEC)	FIRST DERIVATIVE	SECOND DERIVATIVE	
1	1.94839+ 0	1.00000-16	6.48509-16	2.18414-14	
2	1.95754+ 0	1.09005-16	1.01820-15	5.07109-15	
3	1.96532+ 0	1.17234-16	1.05765-15	8.63802-15	
4	1.97398+ 0	1.27041-16	1.13245-15	9.35291-15	
5	1.98327+ 0	1.38369-16	1.21934-15	1.08796-14	
6	1.99163+ 0	1.49323-16	1.31030-15	1.62737-14	
7	1.99581+ 0	1.55084-16	1.37832-15	1.12679-14	
8	2.00000+ 0	1.61057-16			END OF RANGE
9	2.00937+ 0	1.75161-16	1.50525-15	1.23916-14	
10	2.01875+ 0	1.90371-16	1.62148-15	1.32280-14	

H(0) = 2*(1+(F**2)/3!+(F**4)/5!+(F**6)/7!+......
H(1) =-2*F*(1/3+(F**2)/(5*3!)+(F**4)/(7*5!)+(F**6)/(9*7!)+...
H(2) = 2*(1/3+(F**2)/(5*2!)+(F**4)/(7*4!)+(F**6)/(9*6!)+....

11	2.02812+ 0	2.06726-16	1.74543-15	1.40816-14
12	2.03750+ 0	2.24337-16	1.87752-15	1.50120-14
13	2.04687+ 0	2.43247-16	2.01818-15	1.59596-14
14	2.05625+ 0	2.63582-16	2.16788-15	1.69919-14
15	2.06562+ 0	2.85387-16	2.32709-15	1.80414-14
16	2.07500+ 0	3.08802-16	2.49632-15	1.91841-14
17	2.08437+ 0	3.33877-16	2.67608-15	2.03436-14
18	2.09375+ 0	3.60769-16	2.86690-15	2.16056-14
19	2.10312+ 0	3.89528-16	3.06934-15	2.28837-14
20	2.11250+ 0	4.20332-16	3.28399-15	2.42743-14
21	2.12187+ 0	4.53234-16	3.51144-15	2.56800-14
22	2.13125+ 0	4.88431-16	3.75232-15	2.72088-14
23	2.14062+ 0	5.25979-16	4.00727-15	2.87514-14
24	2.15000+ 0	5.66097-16	4.27696-15	3.04287-14
25	2.15937+ 0	6.08844-16	4.56207-15	3.21181-14
26	2.16875+ 0	6.54462-16	4.86334-15	4.21765-14
27	2.17500+ 0	6.86505-16	5.12694-15	2.67052-14
28	2.18750+ 0	7.54765-16	5.46076-15	3.77931-14
29	2.20000+ 0	8.28930-16	5.93317-15	4.05527-14
30	2.21250+ 0	9.09431-16	6.44008-15	4.34740-14
31	2.22500+ 0	9.96724-16	6.98351-15	4.65638-14
32	2.23750+ 0	1.09129-15	7.56555-15	4.98291-14
33	2.25000+ 0	1.19365-15	8.18842-15	5.32770-14
34	2.26250+ 0	1.30433-15	8.85438-15	5.69149-14
35	2.27500+ 0	1.42390-15	9.56582-15	6.07502-14
36	2.28750+ 0	1.55297-15	1.03252-14	6.47904-14
37	2.30000+ 0	1.69215-15	1.11351-14	6.90434-14
38	2.31250+ 0	1.84213-15	1.19981-14	7.35168-14
39	2.32500+ 0	2.00359-15	1.29171-14	7.82188-14
40	2.33750+ 0	2.17728-15	1.38948-14	8.31574-14
41	2.35000+ 0	2.36396-15	1.49343-14	8.83408-14
42	2.36250+ 0	2.56444-15	1.60385-14	9.37774-14
43	2.37500+ 0	2.77957-15	1.72108-14	9.94757-14
44	2.38750+ 0	3.01025-15	1.84542-14	1.05444-13
45	2.40000+ 0	3.25741-15	1.97723-14	1.11691-13
46	2.41250+ 0	3.52201-15	2.11684-14	1.18226-13
47	2.42500+ 0	3.80509-15	2.26462-14	1.25058-13
48	2.43750+ 0	4.10771-15	2.42094-14	1.32194-13
49	2.45000+ 0	4.43098-15	2.58619-14	1.39646-13
50	2.46250+ 0	4.77607-15	2.76075-14	1.47421-13
51	2.47500+ 0	5.14420-15	2.94502-14	1.55528-13
52	2.48750+ 0	5.53663-15	3.13943-14	1.63978-13
53	2.50000+ 0	5.95468-15	3.34440-14	1.72778-13
54	2.51250+ 0	6.39973-15	3.56038-14	1.81940-13
55	2.52500+ 0	6.87320-15	3.78780-14	1.91471-13
56	2.53750+ 0	7.37659-15	4.02714-14	2.01382-13
57	2.55000+ 0	7.91145-15	4.27887-14	2.11682-13
58	2.56250+ 0	8.47939-15	4.54347-14	2.22381-13
59	2.57500+ 0	9.08207-15	4.82145-14	2.33488-13
60	2.58750+ 0	9.72123-15	5.11331-14	2.05829-13
61	2.60625+ 0	1.07523-14	5.49924-14	2.63149-13
62	2.62500+ 0	1.18760-14	5.99264-14	2.82235-13
63	2.64375+ 0	1.30988-14	6.52183-14	3.02347-13
64	2.66250+ 0	1.44279-14	7.08873-14	3.23517-13
65	2.68125+ 0	1.58708-14	7.69532-14	3.45778-13
66	2.70000+ 0	1.74352-14	8.34366-14	3.69162-13
67	2.71875+ 0	1.91295-14	9.03584-14	3.93700-13
68	2.73750+ 0	2.09621-14	9.77402-14	4.19425-13
69	2.75625+ 0	2.29422-14	1.05604-13	4.46367-13
70	2.77500+ 0	2.50792-14	1.13974-13	4.74559-13
71	2.79375+ 0	2.73830-14	1.22872-13	5.04030-13
72	2.81250+ 0	2.98641-14	1.32322-13	5.34810-13
73	2.83125+ 0	3.25331-14	1.42350-13	5.66931-13
74	2.85000+ 0	3.54015-14	1.52980-13	6.00420-13
75	2.86875+ 0	3.84810-14	1.64238-13	6.35308-13

MESSAGE WILL INFORM THE USER THAT CROSS SECTIONS SHOULD BE TABULATED TO HIGHER ENERGIES AND FAILURE TO DO SO MAY LEAD TO ERRONEOUS RESULTS AT HIGHER TEMPERATURES. AFTER PRINTIONG THE WARNING MESSAGE THE PROGRAM WILL PROCEED WITH THE CALCULATION.



THE RUNNING TIME OF THE PROGRAM CAN BE MINIMIZED BY SPECIFYING A NUMBER OF TEMPERATURE RANGES, EACH OF WHICH IS NOT TOO LARGE. IT


```
PLOT TABULATED DATA (PLOTTAB VERSION 87-2)
===================================================================
PLOT CONTINUOUS CURVE.............YES  (TOGETHER - ON ALL PLOTS)
PLOT DISCRETE POINTS..............NO
PLOT SIZE.........................FULL
TYPE OF GRID......................DASHED GRID
SHOULD RATIOS BE PLOTTED..........NO
LINE THICKNESS....................  3
===================================================================
X AXIS LABEL AND UNITS............ Electron Temperature (eV)
Y AXIS LABEL AND UNITS............ Rate Coefficient (cm 3/Sec)
===================================================================
===================================================================
PLOT TITLE
...................................................................
Electron Impact Ionization                      Reaction Rates
      e{- + O{q{+ |2 e{- + O{({q{+{1{){+ + e{-
===================================================================
REQUESTED X RANGE................. PLOT ALL POINTS
PLOT X ERROR BARS.................YES
PLOT Y ERROR BARS.................YES
X PLANE ON PLOTS (IF POSSIBLE)....LOG
Y PLANE ON PLOTS (IF POSSIBLE)....LOG
===================================================================
X LIMITS (PLANE).................. 1.0000E+00  1.0000E+04 (LOG)
Y LIMITS (PLANE).................. 1.0000E-16  9.3736E-08 (LOG)
===================================================================
CONTINUOUS CURVES
...................................................................
INDEX DESCRIPTION                 POINTS
...................................................................
    1 O I -> II      (q = 0)        242
    2 O II -> III    (q = 1)        298
    3 O III -> IV    (q = 2)        281
    4 O IV -> V      (q = 3)        258
    5 O V -> VI      (q = 4)        243
    6 O VI -> VII    (q = 5)        223
    7 O VII -> VIII  (q = 6)        188
    8 O VIII -> IX   (q = 7)        175
===================================================================
END OF RUN       1 PLOTS GENERATED
```

ONCE THE INPUT PARAMETERS AND POSSIBLY TABULATED WEIGHTING HAVE
BEEN READ, ONE TABLE OF CROSS SECTIONS IS READ AND REACTION RATES
ARE CALCULATED AND OUTPUT. THE NEXT TABLE OF CROSS SECTIONS IS
THEN READ AND REACTION RATES ARE CALCULATED AND OUTPUT. THE CYCLE

Program PLOTTAB

```
2.0000D+03 1.0000D-03
4.0000D+03 1.0000D-03
7.0000D+03 1.0000D-03
1.0000D+04 1.0000D-03
```

```
      PROGRAM PLOTTAB(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10,
     1 TAPE11,TAPE12,TAPE14)

      PROGRAM PLOTTAB
      VERSION 87-1 (JANUARY, 1987)
      VERSION 87-2 (MAY, 1987)     *SOFTWARE UPPER AND LOWER CASE
                                    CHARACTERS
                                   *SOFTWARE SPECIAL SYMBOLS TO IDENTIFY
                                    SETS OF DISCRETE POINTS.
                                   *SOFTWARE LINE TYPES TO IDENTIFY
                                    CURVES.

      WRITTEN BY DERMOTT E. CULLEN
                 NUCLEAR DATA SECTION
                 INTERNATIONAL ATOMIC ENERGY AGENCY
                 P.O. BOX 100
                 VIENNA, AUSTRIA
      TELEPHONE  23-60-1718

      PURPOSE
      ===================================================================
      THIS PROGRAM IS DESIGNED TO PLOT ANY COMBINATION OF CONTINUOUS
      CURVES AND/OR DISCRETE POINTS (WITH ASSOCIATED ERROR BARS) USING
      USER SUPPLIED TITLES AND X AND Y AXIS LABELS AND UNITS.

      USING THIS METHOD THE PROGRAM HAS NO IDEA OF WHAT DATA IS BEING
      PLOTTED AND YET BY SUPPLYING TITLES, X AND Y AXIS LABELS AND
      UNITS THE USER CAN PRODUCE ANY NUMBER OF PLOTS WITH EACH PLOT
      CONTAINING ALMOST ANY COMBINATION OF CURVES AND POINTS WITH EACH
      PLOT PROPERLY IDENTIFIED.

      GRAPHICS INTERFACE
      ===================================================================
      THIS PROGRAM USES A SIMPLE CALCOMP LIKE GRAPHICS INTERFACE WHICH
      REQUIRES ONLY 3 SUBROUTINES...PLOTS, PLOT AND PEN (DESCRIBED IN
      DETAIL BELOW). ALL CHARACTERS AND SYMBOLS ARE DRAWN USING TABLES
      OF PEN STROKES (SUPPLIED WITH THIS PROGRAM). USING THIS METHOD
      THE PROGRAM SHOULD BE SIMPLE TO INTERFACE TO VIRTUALLY ANY PLOTTER
      OR GRAPHICS TERMINAL AND THE APPEARANCE AND LAYOUT OF THE PLOTS
      SHOULD BE INDEPENDENT OF WHICH PLOTTER IS USED.

      METHOD
      ===================================================================
      STARTING FROM FILES OF,
      (1) OPTIONS = TO CONTROL SELECTION AND PLOTTING OF DATA.
      (2) CURVES  = IDENTIFIED BY A TITLE AND (X,Y) COORDINATES.
      (3) POINTS  = IDENTIFIED BY A TITLE AND (X,+DX,-DX,Y,+DY,-DY)
                    COORDINATES.

      THIS PROGRAM IS DESIGNED TO CREATE PLOTS OF THE USER SELECTED DATA

      FORMAT OF INPUT OPTIONS, CURVES AND DISCRETE POINTS
      ===================================================================
      THE FORMAT OF ALL FIXED AND FLOATING POINT DATA READ BY THIS
      PROGRAM ARE ALL IN FIELDS 11 COLUMNS WIDE (E.G. I11 OR E11.4)
      WHICH WAS SELECTED TO BE COMPATIBLE WITH THE ENDF/B (EVALUATED
      NUCLEAR DATA) AND EXFOR (EXPERIMENTAL NUCLEAR DATA) FORMATS.
      DATA IN THE ENDF/B OR EXFOR CAN BE EASILY TRANSLATED INTO THE
      FORMATS READ BY THIS PROGRAM.

      OPTIONS
      ===================================================================
```

```
1.36000+ 1 0.00000+ 0
1.36053+ 1 5.76581-20
1.36159+ 1 1.72538-19
     .          .
```

I/O UNIT 4 CONTAINS CONTROL INFORMATION OF TWO TYPES,

GLOBAL PARAMETERS

PARAMETERS WHICH APPLY TO ALL PLOTS, INCLUDING,
(1) WHETHER OR NOT TO PLOT CURVES AND HOW TO GROUP THEM.
(2) WHETHER OR NOT TO PLOT POINTS AND HOW TO GROUP THEM.
(3) THE SIZE OF PLOTS (FULL OR HALF SIZE)
(4) TYPE OF GRID (TICK MARKS, FULL GRID OR DASHED GRID).
(5) WHETHER ONLY DATA SHOULD BE PLOTTED OR DATA AND RATIO OF ALL DATA TO FIRST CURVE.
(6) THE WIDTH OF PLOTTED LINES.
(7) X AND Y AXIS LABELS AND UNITS, E.G., INCIDENT ENERGY (EV) VS. CROSS SECTION (BARNS).

GLOBAL PARAMETERS ARE ONLY READ ONCE, REGARDLESS OF HOW MANY PLOTS ARE PRODUCED.

PLOT PARAMETERS

PARAMETERS WHICH ONLY APPLY TO ONE PLOT, INCLUDING,
(6) A TWO LINE TITLE TO BE CENTERED AND APPEAR AT TOP OF PLOT.
(7) A REQUESTED X RANGE (IF ANY).
(8) WHETHER OR NOT X AND Y ERROR BARS SHOULD TO PLOTTED.
(9) THE X AND Y PLANE OF THE PLOT (LINEAR OR LOG).

PLOTTING IS CONTROLLED BY PLOT PARAMETERS, NOT THE CURVE OR POINT DATA. EACH SET OF PLOT PARAMETERS WILL PRODUCE ONE PLOT. PLOTTING ENDS WHEN ALL SETS OF PLOT PARAMETERS HAVE BEEN READ.

CURVES
===
I/O UNIT 10 CONTAINS INFORMATION DESCRIBING THE CURVES TO BE PLOTTED (IF ANY), INCLUDING,
(1) A ONE LINE TITLE TO IDENTIFY EACH CURVE.
(2) TABULATED (X,Y) PAIRS, ONE PAIR PER LINE, TERMINATED BY A BLANK (NOT 0.0) LINE.

THE SEQUENCE OF CURVE TITLE FOLLOWED BY A TABLE OF VALUES AND TERMINATED BY BLANK MAY BE REPEATED ANY NUMBER OF TIMES TO CREATE A SERIES OF PLOTS.

IF REQUESTED, THE PROGRAM WILL USE THIS DATA TO DRAW CONTINUOUS CURVES CONNECTING THE TABULATED VALUES. EACH CURVE (UP TO 30 MAY APPEAR ON EACH PLOT) WILL BE IDENTIFIED BY ITS TITLE IN A LEGEND BOX TO THE RIGHT OF THE PLOT. FOR EACH PLOT THE TOTAL NUMBER OF DATA POINTS USED TO DEFINE THE CURVE MAY BE UP 6000 (IF THIS IS EXCEEDED ONLY THE FIRST 6000 POINTS WILL BE USED).

POINTS
===
I/O UNIT 11 CONTAINS INFORMATION DESCRIBING THE POINTS TO BE PLOTTED (IF ANY), INCLUDING,
(1) A ONE LINE TITLE TO IDENTIFY EACH SET OF POINTS.
(2) TABULATED (X,+DX,-DX,Y,+DY,-DY) SEXTUPLETS, ONE SEXTUPLET PER LINE, TERMINATED BY A BLANK (NOT 0.0) LINE.

THE SEQUENCE OF POINT TITLE FOLLOWED BY A TABLE OF POINTS AND TERMINATED BY BLANK MAY BE REPEATED ANY NUMBER OF TIMES TO CREATE A SERIES OF PLOTS.

IF REQUESTED, THE PROGRAM WILL USE THIS DATA TO DRAW A SET OF

(BLANK LINE TERMINATES CURVE)

```
O III
 3.07849+ 0 1.00000-16
 3.08750+ 0 1.05425-16
```

DISCRETE POINTS AND ASSOCIATED ERROR BARS (IF REQUESTED). EACH SET OF POINTS (UP TO 30 SETS MAY APPEAR ON EACH PLOT) WILL BE IDENTIFIED BY ITS TITLE IN A LEGEND BOX TO THE RIGHT OF THE PLOT. FOR EACH PLOT THE TOTAL NUMBER OF DISCRETE DATA POINTS MAY BE UP TO 2000 (IF THIS NUMBER IS EXCEEDED ONLY THE FIRST 2000 POINTS WILL BE USED).

COMBINED CURVES AND POINTS

A COMBINATION OF UP TO 30 CURVES AND SETS OF DISCRETE POINTS MAY APPEAR ON EACH PLOT (E.G., IF THERE ARE 10 CURVES THERE CANNOT BE MORE THAN 20 SETS OF DISCRETE POINTS).

OPERATION

THE PROGRAM WILL,

(1) READ ALL GLOBAL PARAMETERS (ONCE)
(2) READ ALL PLOT PARAMETERS
(3) READ ALL REQUESTED CURVE AND/OR POINT DATA (BASED ON GLOBAL PARAMETERS).
(4) DETERMINE THE MINIMUM AND MAXIMUM X AND Y VALUES.
(5) DECIDE WHETHER FOR X AND Y AXIS TO USE LINEAR OR LOG SCALING. LOG SCALING IS USED UNLESS,
    (A) USER INPUT SPECIFIES LINEAR
    (B) THE MINIMUM IS NOT POSITIVE
    (C) THE MAXIMUM IS LESS THAN 10 TIMES THE MINIMUM
(6) IF LINEAR SCALING IS USED FOR THE X AND/OR Y AXIS THE DATA WILL BE SCALED TO OBTAIN AXIS ANNOTATION IN NORMAL FORM TO 3 DIGITS ACCURACY (I.E., IF THE X UNITS ARE EV AND THE MAXIMUM X VALUE IS 0.00350 THE AXIS ANNOTATION WILL BE SCALED TO 3.50 AND THE UNITS MODIFIED TO (10**-3 EV))
(7) PRODUCE A PLOT CONTAINING THE USER SUPPLIED TITLES, X AND Y AXIS LABEL AND UNITS IDENTIFYING EACH CURVE AND SET OF POINTS. THE PLOT WILL ALWAYS CONTAIN THE DATA (CURVES AND/OR DISCRETE POINTS). IF PLOTTING CURVES THE USER MAY OPTIONALLY SPECIFY BY INPUT THAT THE FIRST CURVE IS TO BE USED AS A STANDARD AND THE RATIO OF ALL OTHER DATA (CURVES AND/OR POINTS) TO THE STANDARD SHOULD ALSO APPEAR ON THE PLOT (DATA = TOP 2/3 OF PLOT, RATIO= BOTTOM 1/3 OF PLOT).

THE CYCLE OF STEPS (2)-(7) IS REPEATED UNTIL ALL SETS OF PLOT PARAMETERS HAS BEEN READ.

USING THIS METHOD THE PROGRAM HAS NO IDEA OF WHAT DATA IS BEING PLOTTED AND YET BY SUPPLYING TITLES, X AND Y AXIS LABELS AND UNITS THE USER CAN PRODUCE A SERIES OF PLOTS OF ALMOST COMBINATION OF CURVES AND POINTS WITH EACH PLOT PROPERLY IDENTIFIED.

X ORDER OF DATA

IF ALL DATA IS TO APPEAR ON THE PLOTS (I.E., THE USER DOES NOT SPECIFY AN X RANGE..SEE DESCRIPTION OF INPUT OPTIONS) THE DATA FOR EACH CURVE OR SET OF DISCRETE POINTS MAY BE IN ANY X ORDER, E.G., THE POINTS FOR A CURVE MAY BE ASCENDING OR DESCENDING ORDER OR MAY EVEN REVERSE IN X.

IF YOU WISH TO SPECIFY X RANGES OR HAVE RATIOS ON A PLOT THE DATA FOR EACH CURVE OR SET OF DISCRETE POINTS MUST BE IN ASCENDING (DISCONTINUITY ALLOWED) X ORDER. FAILURE TO CONFORM TO THIS RULE CAN RESULT IN UNPREDICTABLE RESULTS.

INTERPOLATION OF CURVES

IN ORDER TO DEFINE A CONTINUOUS CURVE THE PROGRAM ASSUMES LINEAR VARIATION IN X AND Y BETWEEN TABULATED POINTS. FOR A PLOT WHICH IS SCALED TO BE LINEAR IN X AND Y THIS ASSUMPTION CORRESPONDS TO DRAWING A STRAIGHT LINE BETWEEN POINTS ON THE PLOT. IF EITHER OR BOTH AXIS ARE SCALED TO LOG THE PROGRAM WILL INTERPOLATE BETWEEN TABULATED VALUES TO PRESENT A SMOOTH CURVE BETWEEN TABULATED POINTS CORRESPONDING TO LINEAR VARIATION BETWEEN TABULATED POINTS.

TABULATED POINTS SHOULD BE TABULATED AT A SUFFICIENT NUMBER OF X VALUES TO INSURE THAT THE DIFFERENCE BETWEEN LINEAR VARIATION AND THE 'TRUE' VARIATION BETWEEN TABULATED POINTS IS RELATIVELY SMALL.

FOR SOME APPLICATIONS THIS CAN BE VERY IMPORTANT, E.G., CONSIDER THE CASE WHEN WE HAVE THE SIMPLE FUNCTION Y=1/X. TRY COMPARING THE RESULTS OBTAINED AT X=500.0 FOR,

(1) THE EXACT VALUE.....Y=1/500.=0.002

(2) THE RESULT OBTAINED BY ONLY TABULATING THE FUNCTION AT X=1.0 (Y=1.0) AND X=1000.0 (Y=0.001) AND LINEARLY INTERPOLATING BETWEEN THESE 2 VALUES.....Y=ABOUT 0.5

(3) THE RESULTS OBTAINED BY TABULATING THE FUNCTION AT X=1.0 UP TO X=1000.0 USING STEPS IN X OF 1.0.....Y=0.002

IN (2) WHERE AN INSUFFICIENT NUMBER OF POINTS WERE USED THE PREDICTED Y IS A FACTOR OF 250 TOO HIGH. IF THIS TABULATED DATA IS EVER USED IN AN INTEGRAL THE INTEGRAL OF THE DATA IN (2) IS ABOUT 500. WHEREAS THE EXACT INTEGRAL IS ABOUT 6.9 (THE CASE (2) INTEGRAL IS OVER 70 TIMES TOO HIGH).

THE ABOVE EXAMPLE IS NATURALLY AN EXTREME EXAMPLE, BUT HOPEFULLY IT ILLUSTATES THE PROBLEMS WHICH CAN OCCUR WHEN TRYING TO PRODUCE ACCURATE CURVES FROM TABULATED VALUES.

IF YOU HAVE A FUNCTION WHICH YOU WISH TO TABULATE AND YOU ARE NOT SURE HOW MANY TABULATED VALUES TO USE AND WHERE TO LOCATE THEM CONTACT THE AUTHOR FOR A COPY OF PROGRAM LINTAB, WHICH IS DESIGNED TO START FROM ANY USER SUPPLIED FUNCTION AND TO CREATE A TABLE OF LINEARLY INTERPOLABLE POINTS TO WITHIN ANY USER DESIRED ACCURACY.

I/O UNITS

UNIT	DESCRIPTION
4	INPUT OPTIONS (NOTE, UNIT 5 IS RESERVED FOR KEYBOARD INTERACTION ON AN IBM-PC).
6	OUTPUT REPORT
10	TITLES AND SETS OF POINTS FOR EACH CURVE.
11	TITLES AND SETS OF DISCRETE POINTS.
12	SOFTWARE CHARACTER TABLE
14	SOFTWARE SYMBOL AND LINE TYPE TABLE

INPUT OPTIONS (ON I/O UNIT 4)

GLOBAL PARAMETERS

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-11	I11	SHOULD CURVES BY PLOTTED, = 0 - NO = 1 - YES..1 CURVE PER PLOT. = 2 - YES..ALL CURVES ONLY ON FIRST PLOT. (UP TO 30 CURVES)

			= 3 - YES..ALL CURVES ON ALL PLOTS. (UP TO 30 CURVES)
	12-22	I11	SHOULD POINTS BY PLOTTED, = 0 - NO = 1 - YES..1 SET OF POINTS PER PLOT. = 2 - YES..ALL SETS ONLY ON FIRST PLOT. (UP TO 30 SETS) = 3 - YES..ALL SETS ON ALL PLOTS. (UP TO 30 SETS)
	23-33	I11	PLOT SIZE = 0 - FULL (1 PLOT PER PAGE) = 1 - HALF (4 PLOTS PER PAGE)
	34-44	I11	TYPE OF GRID ON PLOTS = 0 - TICK MARKS ON BORDER OF PLOT. = 1 - FULL GRID LINES ACROSS PLOT. = 2 - DASHED GRID LINES ACROSS PLOT.
	45-55	I11	SHOULD RATIO OF ALL DATA TO FIRST CURVE BE PLOTTED. = 0 - NO = 1 - YES
	56-66	I11	SHOULD CURVES BE DRAWN NORMAL WIDTH OR THICKER. = 0 - NORMAL = 1 TO 10 - LINE THICKNESS
2	1-40	40A1	X LABEL LABEL, E.G. INCIDENT ENERGY
	41-72	32A1	X LABEL UNITS, E.G. EV (NOTE, ON THE PLOT THE PROGRAM WILL PLOT PARENTHESIS AROUND THE UNITS).
3	1-40	40A1	Y LABEL LABEL, E.G. CROSS SECTION
	41-72	32A1	Y LABEL UNITS, E.G. BARNS (NOTE, ON THE PLOT THE PROGRAM WILL PLOT PARENTHESIS AROUND THE UNITS).

THE ABOVE 3 LINES ARE ONLY READ ONCE (I.E. IT IS NOT READ FOR EACH PLOT)

PLOT PARAMETERS

LINE	COLUMNS	FORMAT	DESCRIPTION
4	1-72	72A1	FIRST LINE OF TITLE (FOR TOP OF PLOT)
5	1-72	72A1	SECOND LINE OF TITLE (FOR TOP OF PLOT)
6	1-11	E11.4	MINIMUM X LIMIT OF PLOT (BLANK INDICATES NO LIMIT...USE MINIMUM X VALUE OF DATA).
	12-22	E11.4	MAXIMUM X LIMIT OF PLOT (BLANK INDICATES NO LIMIT...USE MAXIMUM X VALUE OF DATA).
	23-33	I11	SHOULD X ERROR BARS BE PLOTTED. = 0 - NO = 1 - YES
	34-44	I11	SHOULD Y ERROR BARS BE PLOTTED. = 0 - NO = 1 - YES
	45-55	I11	X AXIS SCALING = 1 - LINEAR (SCALED TO LOWER DATA LIMIT) =-1 - LINEAR (SCALED TO LOWER 0.0 LIMIT) = OTHERWISE DEFAULT OF LOG
	56-66	I11	Y AXIS SCALING = 1 - LINEAR (SCALED TO LOWER DATA LIMIT) =-1 - LINEAR (SCALED TO LOWER 0.0 LIMIT) = OTHERWISE DEFAULT OF LOG

THE ABOVE 3 LINES ARE READ FOR EACH PLOT. PROGRAM EXECUTION

12	[illegible]	[illegible]	[illegible]	[illegible]
13	1.07500+ 0	2.63458-14	3.09166-13	3.28417-12
14	1.08125+ 0	2.84064-14	3.29693-13	3.45767-12
15	1.08750+ 0	3.06020-14	3.51303-13	3.63773-12
16	1.09375+ 0	3.29397-14	3.74039-13	3.82447-12

TERMINATES AT THE END OF INPUT.

NOTE, IF THE MINIMUM X VALUE IS NOT LESS THAN THE MAXIMUM X VALUE THE PLOT WILL BE SCALED TO CONTAIN ALL DATA (SEE, EXAMPLE 1. AND 2., BELOW)

NOTE, REGARDLESS OF WHETHER OR NOT THE POINTS INCLUDE UNCERTAINTY (+DX,-DX,+DY,-DY) COLUMNS 34-44 AND 45-55 OF INPUT LINE 6 CONTROL WHETHER OR NOT THE UNCERTAINTY IS CONSIDERED IN SCALING THE PLOT AND WHETHER OR NOT ERROR BARS WILL APPEAR ON THE PLOT.

GROUPING DATA ON PLOTS
==

BY USING INPUT OPTIONS THE USER HAS CONTROL OVER HOW MANY SETS OF CURVES AND/OR POINTS WILL APPEAR ON EACH PLOT. ON THE FIRST INPUT LINE COLUMNS 1-11 CONTROL HOW CURVES SHOULD APPEAR ON EACH PLOT AND COLUMNS 12-22 CONTROL HOW POINTS SHOULD APPEAR ON EACH PLOT. THESE OPTIONS CONTROL HOW MANY SETS (IF ANY) OF A GIVEN TYPE OF DATA (CURVES OR POINTS) WILL BE READ OR KEPT IN CORE FOR THE NEXT PLOT. THE AVAILABLE OPTIONS ARE,

(0) DATA IS NOT TO BE READ OR APPEAR ON PLOT. WHEN YOU WISH TO PLOT ONE TYPE OF DATA (CURVES OR POINTS) THIS OPTION SHOULD BE SPECIFIED FOR THE OTHER TYPE OF DATA. YOU CANNOT SPECIFY THIS OPTION FOR BOTH TYPES OF DATA. IF YOU DO THE PROGRAM WILL SIMPLY TELL YOU THAT YOU ARE NOT REQUESTING ANY PLOTS AND TERMINATE. E.G., IF YOU WISH TO ONLY PLOT CURVES SPECIFY THIS OPTION FOR POINTS (COLUMNS 12-22 = 0).

(1) FOR THE NEXT PLOT READ THE NEXT SET OF DATA (POINTS OR CURVES) AND USE IT ONLY FOR THE NEXT PLOT. THIS OPTION MAY BE USED WHEN YOU WISH TO CREATE A SERIES OF PLOTS EACH CONTAINING ONLY ONE SET OF A TYPE OF DATA (POINTS OR CURVES) PLUS ANY NUMBER (0 TO 30) OF SETS OF THE OTHER TYPE OF DATA. NOTE, THE SET OF DATA WILL ONLY APPEAR ON ONE PLOT, SO THAT YOU CANNOT FIRST SPECIFY THE ENTIRE X RANGE FOR ONE PLOT AND THEN SPECIFY A MINIMUM AND MAXIMUM RANGE FOR A SECOND PLOT. E.G., IF YOU WISH TO CREATE A SERIES OF PLOTS EACH CONTAINING ONLY ONE CURVE SPECIFY THIS OPTION FOR CURVES (COLUMNS 1-11 = 1).

(2) FOR THE FIRST PLOT READ ALL SETS OF DATA (POINTS OR CURVES) AND USE IT ONLY FOR THE NEXT PLOT. THIS OPTION MAY BE USED WHEN YOU WISH ALL OF THE DATA OF A GIVEN TYPE (CURVES OR POINTS) TO ONLY APPEAR ON THE FIRST PLOT. NOTE, THE DATA WILL ONLY APPEAR ON THE FIRST PLOT, SO THAT YOU CANNOT FIRST PLOT THE ENTIRE X RANGE FOR ONE PLOT AND THEN SPECIFY A MINIMUM AND MAXIMUM RANGE FOR A SECOND PLOT. E.G., IF YOU WISH TO CREATE A SERIES OF PLOTS OF CURVES WITH ALL POINTS ONLY ON THE FIRST PLOT SPECIFY THIS OPTION FOR POINTS (COLUMNS 12-22 = 2).

(3) READ ALL DATA (POINTS OR CURVES) AND USE IT FOR ALL PLOTS. THIS OPTION MAY BE USED IF YOU WISH TO CREATE A SERIES OF PLOTS EACH CONTAINING ALL OF THE DATA OF A GIVEN TYPE. NOTE, IN THIS CASE YOU MAY FIRST PLOT THE ENTIRE X RANGE AND THEN SPECIFY MINIMUM AND MAXIMUM RANGES FOR ANY NUMBER OF FOLLOWING PLOTS. E.G., IF YOU WISH TO A CREATE A SERIES OF PLOTS EACH CONTAINING ALL OF THE CURVES AND EACH INVOLVING A DIFFERENT X RANGE SPECIFY THIS OPTION FOR CURVES (COLUMNS 1-11 = 3).

IN ORDER TO CREATE OTHER COMBINATIONS OF CURVES AND PLOTS IT IS USUALLY EASIER TO EDIT YOUR CURVE AND POINT FILES TO CONTAIN THE THE DATA TO APPEAR ON THE PLOTS THAN TO INCLUDE MORE INPUT OPTIONS

77	[illegible]	[illegible]	[illegible]	
78	1.86091+ 0	6.82730-12	2.74795-11	7.95367-11
79	1.88589+ 0	7.56336-12	2.94663-11	1.01322-10
80	1.90681+ 0	8.22414-12	3.15860-11	9.14179-11
81	1.93010+ 0	9.00937-12	3.37151-11	1.16496-10

IN THIS PROGRAM. E.G., IF YOU HAVE A SERIES OF CURVES AND YOU WISH TO PLOT EACH SEPARATELY, BUT YOU WOULD LIKE A SERIES OF PLOTS OF DIFFERENT X RANGES FOR EACH CURVE, CREATE A NUMBER OF CURVE FILES EACH CONTAINING ONLY ONE CURVE AND RUN EACH FILE SEPARATELY WITH COLUMNS 1-11 = 3.

PLOTTING RATIOS
===

WHICHEVER DATA IS REQUESTED (CURVES AND/OR POINTS) WILL ALWAYS BE PLOTTED. WHEN PLOTTING CURVES THE USER HAS THE OPTION TO USE THE FIRST CURVE AS A STANDARD AND TO PLOT NOT ONLY THE DATA (UPPER 2/3 OF PLOT), BUT ALSO THE RATIO OF ALL CURVES AND/OR DATA POINTS TO THE STANDARD (LOWER 1/3 OF PLOT). THIS OPTION IS EXTREMELY HANDY WHEN YOU WOULD LIKE TO QUANTITATELY DEFINE THE AGREEMENT BETWEEN CURVES AND/OR POINTS (E.G., IT IS EASY TO SEE FROM THE PLOT THAT 2 CURVES DIFFER BY 15 PER-CENT).

EXAMPLE NO. 1 UNIT 4 INPUT

PLOT EACH CURVE SEPARATELY, PLOT ALL POINTS ON ALL PLOTS, CREATE FULL SIZED PLOTS WITH TICK MARKS ON THE BORDER, USE THE BELOW INDICATED X AND Y AXIS LABELS AND UNITS. IF UNIT 10 CONTAINS THE 27-CO-59 (N,2N) ENDF/B-IV, JENDL-II AND ENDL84 EVALUATIONS AND UNIT 11 CONTAINS ALL OF THE EXPERIMENTAL DATA THE BELOW INPUT WILL CREATE 3 SEPERATE PLOTS EACH PLOT CONTAINING 1 EVALUATION AND ALL EXPERIMENTAL DATA (SEE, UNIT 10 EXAMPLE BELOW TO ILLUSTRATE HOW THE PROGRAM IDENTIFIES EACH EVALUATION).

```
          1          3          0          0          0          0
INCIDENT ENERGY                            EV
CROSS SECTION                              BARNS
27-CO-59                                                   (N,2N)
CROSS SECTIONS
                                1          1          0          0
27-CO-59                                                   (N,2N)
CROSS SECTIONS
                                1          1          0          0
27-CO-59                                                   (N,2N)
CROSS SECTIONS
                                1          1          0          0
```

EXAMPLE NO. 2 UNIT 4 INPUT

PLOT ALL CURVES ON ONE, PLOT ALL POINTS ON ONE PLOT, CREATE FULL SIZED PLOTS WITH TICK MARKS ON THE BORDER, USE THE BELOW INDICATED X AND Y AXIS LABELS AND UNITS. IF UNIT 10 CONTAINS THE 27-CO-59 (N,2N) ENDF/B-IV, JENDL-II AND ENDL84 EVALUATIONS AND UNIT 11 CONTAINS ALL OF THE EXPERIMENTAL DATA THE BELOW INPUT WILL CREATE 1 PLOT COMPARING ALL EVALUATIONS AND ALL EXPERIMENTAL DATA (SEE, UNIT 10 EXAMPLE BELOW TO ILLUSTRATE HOW PROGRAM IDENTIFIES EACH EVALUATION).

```
          3          3          0          0          0          0
INCIDENT ENERGY                            EV
CROSS SECTION                              BARNS
27-CO-59                                                   (N,2N)
CROSS SECTIONS
                                1          1          0          0
```

EXAMPLE NO. 3 UNIT 4 INPUT

TO COMPARE THE ENDF/B-IV 27-CO-59 (N,2N) EVALUATION TO ALL

```
143  7.00000+ 0  3.04564- 9                                 END OF RANGE
144  7.30000+ 0  3.39522- 9  1.16529- 9  1.14429-10
145  7.75000+ 0  3.94278- 9  1.21678- 9  1.22064-10
146  8.20000+ 0  4.51505- 9  1.27171- 9  9.14610-11
```

EXPERIMENTAL DATA OVER THE ENERGY RANGE 15 TO 20 MEV AND USING THE SAME PLOT OPTIONS AS ABOVE THE BELOW INPUT WILL CREATE 1 PLOT CONTAINING ENDF/B-IV AND ALL EXPERIMENTAL DATA (SEE, UNIT 10 EXAMPLE BELOW TO ILLUSTRATE HOW PROGRAM IDENTIFIES ENDF/B-IV).

```
         3          3          0          0          0          0
INCIDENT ENERGY                          EV
CROSS SECTION                            BARNS
27-CO-59                                                    (N,2N)
CROSS SECTIONS
 1.50000+ 7 2.00000+ 7         1          1          0          0
```

EXAMPLE NO. 4 UNIT 4 INPUT

TO COMPARE THE ENDF/B-IV 27-CO-59 TOTAL (N,N'), (N,2N) AND (N,3N) CROSS SECTIONS OVER THE ENERGY RANGE 10 TO 20 MEV PREPARE THESE 3 SETS OF DATA AS SEPARATE CURVES ON THE CURVE FILE (UNIT 10) IN THE ORDER (N,N'), (N,2N) FOLLOWED BY (N,3N) IDENTIFYING EACH REACTION BY THE TITLE LINE. PLOT NOT ONLY THE CROSS SECTIONS BUT ALSO THE RATIOS (N,2N)/(N,N') AND (N,3N)/(N,N') (NOTE, THE DENOMINATOR IN THESE RATIO WILL BE THE FIRST CURVE DEFINED ON THE CURVE FILE).

```
         3          0          0          0          1          0
INCIDENT ENERGY                          EV
CROSS SECTION                            BARNS
27-CO-59                                              ENDF/B-IV
CROSS SECTIONS
 1.00000+ 7 2.00000+ 7         1          1          0          0
```

CURVE DATA (ON I/O UNIT 10)
===

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-26	26A1	TITLE FOR CURVE
2-N	1-11	E11.4	X VALUE
	12-22	E11.4	Y VALUE

EACH CURVE IS TERMINATED BY BLANK (NOT 0.0). THE SEQUENCE OF TITLE FOLLOWED BY TABULATED POINTS MAY BE REPEATED ANY NUMBER OF TIMES. EACH PLOT MAY CONTAIN UP TO 6000 POINTS.

EXAMPLE UNIT 10 INPUT

IF UNIT 10 CONTAINS THE 27-CO-59 (N,2N) EVALUATIONS FROM ENDF/B-IV JENDL-II AND ENDL84 THE DATA COULD LOOK LIKE,

```
ENDF/B-IV                                       27-CO-59 (N,2N)
 1.10000+ 7 0.00000+ 0
 1.20000+ 7 1.20000- 3
      .          .
      .          .
 2.00000+ 7 3.00000- 2
                         (NOTE, BLANK CARD TERMINATES CURVE).
JENDL-II                                        27-CO-59 (N,2N)
 1.07000+ 7 0.00000+ 0
 1.16000+ 7 1.13000- 3
      .          .
      .          .
 2.00000+ 7 2.80000- 2
                         (NOTE, BLANK CARD TERMINATES CURVE).
ENDL84                                          27-CO-59 (N,2N)
 1.12000+ 7 0.00000+ 0
```

```
207  7.90000+ 2  [illegible]
208  8.05000+ 2  9.10338- 8 -1.02363-11 -3.66322-15
209  8.20000+ 2  9.08794- 8 -1.02912-11 -3.01280-15
210  8.35000+ 2  9.07243- 8 -1.03364-11 -2.41988-15
```

```
1.22000+ 7 1.27000- 3
    .          .
    .          .
2.00000+ 7 2.90000- 2
                           (NOTE, BLANK CARD TERMINATES CURVE).
```

NOTE, FOR IDENTIFICATION ON EACH PLOT THE PROGRAM WILL ONLY READ AND USE THE FIRST 26 CHARACTERS OF THE TITLE. THE USER MAY USE THE REMAINDER OF THE TITLE LINE TO FURTHER PHYSICALLY IDENTIFY THE DATA.

NOTE, THE ABOVE DATA IS FOR ILLUSTRATION PURPOSES ONLY AND DOES NOT CORRESPOND TO THE ACTUAL DATA FROM THESE EVALUATED LIBRARIES.

POINT DATA (ON I/O UNIT 11)

LINE	COLUMNS	FORMAT	DESCRIPTION
1	1-26	26A1	TITLE FOR CURVE
2-N	1-11	E11.4	X VALUE
	12-22	E11.4	POSITIVE X UNCERTAINTY
	23-33	E11.4	NEGATIVE X UNCERTAINTY
	34-44	E11.4	Y VALUE
	45-55	E11.4	POSITIVE Y UNCERTAINTY
	55-66	E11.4	NEGATIVE Y UNCERTAINTY

EACH SET OF POINTS IS TERMINATED BY BLANK (NOT 0.0). THE SEQUENCE TITLE FOLLOWED BY TABULATED POINTS MAY BE REPEATED ANY NUMBER OF TIMES. EACH PLOT MAY CONTAIN UP TO 2000 POINTS.

UNCERTAINTIES

UNCERTAINTIES MUST BE IN THE SAME UNITS AS THE DATA (E.G., EV OR BARNS). THE UNCERTAINTIES WILL BE INTERPRETED TO DEFINE THE ERROR BARS RELATIVE TO THE DATA POINT. THE ERROR BARS FOR A POINT WILL EXTEND FROM THE POINT MINUS THE NEGATIVE ERROR TO THE POINT PLUS THE POSITIVE ERROR (E.G., 10 BARNS +/- 2 BARNS DEFINES AN ERROR BAR FROM 8 TO 12 BARNS). NEVER TRY TO USE THE UNCERTAINTIES TO DIRECTLY DEFINE THE ERROR BARS (E.G., IN THE ABOVE EXAMPLE YOU CANNOT DEFINE THE UNCERTAINTIES AS 8 AND 12 BARNS).

THE UNCERTAINTIES CAN BE SYMMETRIC OR NON-SYMMETRIC AND CAN BE GIVEN OR SIMPLY LEFT BLANK (NO UNCERTAINTY GIVEN). NOTE, FOR A SYMMETRIC UNCERTAINTY YOU MUST ENTER BOTH A POSITIVE AND NEGATIVE UNCERTAINTIES.

IT DOES NOT MATTER WHETHER YOU DEFINE THE UNCERTAINTIES TO BE POSITIVE OR NEGATIVE ON UNIT 11 (YOU CAN USE ANY CONVENTION THAT YOU LIKE). INTERNALLY THE PROGRAM WILL DEFINE ALL UNCERTAINTIES TO BE POSITIVE NUMBERS AND USE THE UNCERTAINTIES TO DEFINE A POSITIVE ERROR BAR (EXTENDING FROM THE POINT TO THE POINT PLUS THE POSITIVE ERROR) AND A NEGATIVE ERROR BAR (EXTENDING FROM THE POINT TO THE POINT MINUS THE NEGATIVE ERROR).

EXAMPLE UNIT 11 INPUT

IF UNIT 11 CONTAINS THE EXPERIMENTAL MEASURED DATA 27-CO-59 (N,2N) THE DATA COULD LOOK LIKE,

```
L.R.VEESER, ET AL. (77)                               27-CO-59 (N,2N)
 1.10000+ 7 1.10000+ 6 1.10000+ 6 1.10000- 4 2.30000- 4 1.10000- 4
 1.20000+ 7                       1.20000- 3
```

```
  7  1.99581+ 0  1.55084-16  1.37832-15  1.12679-14
  8  2.00000+ 0  1.61057-16                          END OF RANGE
  9  2.00937+ 0  1.75161-16  1.50525-15  1.23916-14
 10  2.01875+ 0  1.90371-16  1.62148-15  1.32280-14
```

```
     .         .
     .         .
 2.00000+ 7 2.20000+ 6 2.20000+ 6 3.00000- 2
                             (NOTE, BLANK CARD TERMINATES DATA SET).
S.OKAMURA (67)                                 27-CO-59 (N,2N)
 1.07000+ 7 1.07000+ 6 1.07000+ 6 1.30000- 4 3.40000- 4 1.10000- 4
 1.16000+ 7                       1.40000- 3
     .         .
     .         .
 2.00000+ 7 2.20000+ 6 2.20000+ 6 3.10000- 2
                             (NOTE, BLANK CARD TERMINATES DATA SET).
A.PAULSEN, ET AL (65)                           27-CO-59 (N,2N)
 1.13000+ 7 1.13000+ 6 1.13000+ 6 1.80000- 4 3.40000- 4 1.10000- 4
 1.37000+ 7                       2.80000- 3
     .         .
     .         .
 2.00000+ 7 2.20000+ 6 2.20000+ 6 3.30000- 2
                             (NOTE, BLANK CARD TERMINATES DATA SET).
     .         .
     .         .
(NOTE, ANY NUMBER OF REFERENCES MAY FOLLOW)
```

NOTE, FOR IDENTIFICATION ON EACH PLOT THE PROGRAM WILL ONLY READ AND USE THE FIRST 26 CHARACTERS OF THE TITLE. THE USER MAY USE THE REMAINDER OF THE TITLE LINE TO FURTHER PHYSICALLY IDENTIFY THE DATA.

NOTE, THE ABOVE DATA IS FOR ILLUSTRATION PURPOSES ONLY AND DOES NOT CORRESPOND TO THE ACTUAL DATA FROM THESE REFERENCES.

ON WHAT COMPUTERS WILL THE PROGRAM RUN
==
THE PROGRAM HAS BEEN IMPLEMENTED ON AN IBM MAINFRAME AND AN IBM-AT PERSONAL COMPUTER WITH AN ATTACHED HEWLETT-PACKARD 7475A PLOTTER. THE PROGRAM IS SMALL ENOUGH TO RUN ON VIRTUALLY ANY COMPUTER. FOR SPECIAL CONSIDERATIONS SEE THE SECTIONS BELOW ON
(1) COMPUTER DEPENDENT CODING
(2) PLOTTER/GRAPHICS TERMINAL INTERFACE

THE PROGRAM CAN DETERMINE WHETHER IT IS RUNNING ON A MAINFRAME OR AN IBM-PC. THE VARIABLE IBMPC IS INITIALIZED TO -1. IF RUNNING ON A MAINFRAME ITS VALUE WILL WILL NOT CHANGE. IF RUNNING ON AN IBM-PC THE PLOTTER INTERFACE ROUTINE PLOTS WILL RESET IBMPC TO,

IBMPC = 0 - IBM-PC FULL SIZE PLOTS
IBMPC = 1 - IBM-PC HALF SIZE PLOTS

KNOWING WHETHER THE PROGRAM IS EXECUTING ON A MAINFRAME OR IBM-PC CAN BE USED BY THE PROGRAM TO OPTIMIZE EXECUTION.

REPORTING ERRORS
==
IN ORDER TO IMPROVE THIS CODE AND MAKE FUTURE VERSIONS MORE COMPATIBLE FOR USE ON AS MANY DIFFERENT TYPES OF COMPUTERS AS POSSIBLE PLEASE REPORT ALL COMPILER DIAGNOSTICS AND/OR OPERATING PROBLEMS TO THE AUTHOR AT THE ABOVE ADDRESS.

PLEASE REMEMBER IF YOU SIMPLY REPORT 'I'VE GOT A PROBLEM' AND DO NOT ADEQUATELY DESCRIBE EXACTLY HOW YOU WERE USING THE PROGRAM IT WILL BE IMPOSSIBLE FOR THE AUTHOR TO HELP YOU. WHEN A PROBLEM ARISES PLEASE WRITE TO THE AUTHOR, DESCRIBE THE PROBLEM IN AS MUCH DETAIL AS POSSIBLE, IDENTIFY THE VERSION OF THE PROGRAM THAT YOU

72	2.81250+ 0	2.98641-14	1.32322-13	5.34810-13
73	2.83125+ 0	3.25331-14	1.42350-13	5.66931-13
74	2.85000+ 0	3.54015-14	1.52980-13	6.00420-13
75	2.86875+ 0	3.84810-14	1.64238-13	6.35308-13

ARE USING (E.G. VERSION 87-2) AND SEND THE FOLLOWING INFORMATION ON MAGNETIC TAPE TO THE AUTHOR,

(1) A COPY OF THE FORTRAN PROGRAM YOU ARE USING
(2) A COPY OF COMPILER DIAGNOSTICS (IF ANY)
(3) A COPY OF YOUR JCL AND INPUT OPTIONS (UNIT 4)
(4) A COPY OF YOUR CURVE DATA (UNIT 10)
(5) A COPY OF YOUR POINT DATA (UNIT 11)
(6) A COPY OF SOFTWARE CHARACTER TABLE (UNIT 12)
(7) A COPY OF SOFTWARE SYMBOL AND LINE TYPE TABLE (UNIT 14)
(8) A COPY OF THE OUTPUT REPORT FROM THE PROGRAM (UNIT 6)
(9) A COPY OF THE PLOTS FROM THE PROGRAM

WITHOUT ALL OF THIS INFORMATION IT IS IMPOSSIBLE TO EXACTLY SIMULATE THE PROBLEM THAT YOU RAN AND TO DETERMINE THE SOURCE OF YOUR PROBLEM.

***** COMPUTER DEPENDENT CODING **

* THIS PROGRAM IS DESIGNED TO BE USED WITH A FORTRAN-77 COMPILER.

* THE ONLY COMPILER DEPENDENT FORMAT STATEMENTS INVOLVE,
  (1) CHARACTER*1 AND CHARACTER*4
  (2) TESTING FOR ERRORS AND END OF FILE DURING READS.

* IT IS ASSUMED THAT CHARACTERS ARE STORED IN SUCCESSIVE BYTE LOCATIONS AND THAT CHARACTERS MAY BE TREATED AS CONTINUOUS STRINGS OF CHARACTERS IN EITHER CHARACTER*4 OR CHARACTER*1 FORMAT.

* FOR EXAMPLE, IF ONE SUBROUTINE CONTAINS,

```
CHARACTER*4 BCD
DIMENSION BCD(10)
```

THE ARRAY BCD IS ASSUMED TO BE AN ARRAY OF 40 CHARACTERS IN SUCCESSIVE BYTE LOCATIONS.

IT IS ASSUMED THAT THIS ARRAY CAN BE PASSED AS AN ARGUMENT TO ANOTHER SUBROUTINE AND USED AS CHARACTER*1,E.G.,

```
CALL DUMMY(BCD)

SUBROUTINE DUMMY(BCD)
CHARACTER*1 BCD
DIMENSION BCD(40)
```

* THIS CONVENTION WILL WORK ON ALL 32 BIT PER WORD COMPUTERS (E.G., IBM OR IBM COMPATIBLE COMPUTERS).

* FOR LONGER WORD LENGTH COMPUTERS (E.G., CDC OR CRAY) IT IS SUGGESTED THAT BEFORE IMPLEMENTING AND USING THIS PROGRAM THE USER FIRST VERIFY THAT CHARACTER STRINGS CAN BE TREATED AS DESCRIBED ABOVE, E.G., WRITE A SIMPLE PROGRAM TO READ A CHARACTER STRING OF 40 CHARACTERS IN CHARACTER*4 FORMAT, PASS IT TO A SUBROUTINE WHICH USES THE CHARACTER STRING IN CHARACTER*1 FORMAT AND PRINT THE CHARACTER STRING IN THE SUBROUTINE. IF THE CHARACTER STRING IS PRINTED AS A CONTINUOUS STRING YOU WILL BE ABLE TO USE THIS PROGRAM. IF THE CHARACTER STRING IS NOT PRINTED AS A CONTINUOUS STRING IT IS NOT RECOMMENDED THAT YOU USE THIS PROGRAM.

* THIS PROGRAM USING THE FORTRAN-77 CONVENTION FOR TESTING FOR READING ERRORS AND END OF FILE DURING READS, E.G.,

```
      READ(10,1000,END=100,ERR=200) A,B,C,D

***** COMPUTER DEPENDENT CODING *****************************************
***** PLOTTER/GRAPHICS TERMINAL INTERFACE *******************************

       THIS PROGRAM USES A SIMPLE CALCOMP LIKE INTERFACE INVOLVING
       ONLY 3 SUBROUTINES,

       PLOTS(BUF,IBUF,IPLOT) - INITIALIZE PLOTTER
             BUF    - PLOTTER BUFFER
             IBUF   - SIZE OF PLOTTING BUFFER (5000 WORDS USED)
             IPLOT  - PLOTTER UNIT (16)...USUALLY A DUMMY UNIT

       PLOT(X,Y,IPEN)          - DRAW OR MOVE FROM LAST LOCATION TO (X,Y),
                                 END OF CURRENT PLOT OR END OF PLOTTING.
             IPEN =   2 - DRAW
                  =   3 - MOVE
                  =  -1 - END OF CURRENT PLOT...ADVANCE BY X,Y
                  = 999 - END OF PLOTTING.

       PEN(IPEN)               - SELECT COLOR.
            IPEN- COLOR = 1 TO N (N = ANY POSITIVE INTEGER)

      IN ORDER TO INTERFACE THIS PROGRAM FOR USE ON ANY PLOTTER WHICH
      DOES NOT USE THE ABOVE CONVENTIONS IT IS MERELY NECESSARY FOR THE
      THE USER TO WRITE 3 SUBROUTINES WITH THE NAMES PLOTS, PLOT AND PEN
      WITH THE SUBROUTINE ARGUMENTS DESCRIBED ABOVE AND TO THEN CALL THE
      LOCAL EQUIVALENT ROUTINES.

      AVAILABLE PLOTTER INTERFACES
      ==================================================================
      THIS PROGRAM HAS AVAILABLE PLOTTER INTERFACES TO OPERATE AS
      FOLLOWS,
      (1) MAINFRAME - HARDCOPY PLOTS IN BLACK AND WHITE.
      (2) MAINFRAME - SCREEN PLOTS IN 7 COLORS ON IBM GRAPHICS TERMINAL.
      (3) IBM-PC    - HARDCOPY PLOTS IN 6 COLORS ON A HEWLETT-PACKARD
                      7475A PLOTTER.

      CONTACT THE AUTHOR TO OBTAIN COPIES OF ANY OF THE ABOVE PLOTTER
      INTERFACES.

      COLOR PLOTS
      ==================================================================
      TO SELECT PLOTTING COLORS SUBROUTINE PEN (DESCRIBED ABOVE) IS USED
      TO SELECT ONE OF THE AVAILABLE COLORS. WHEN RUNNING ON A MAINFRAME
      USING AN IBM GRAPHICS TERMINAL OR ON AN IBM-PC USING A HEWLETT-
      PACKARD PLOTTER THE GRAPHICS INTERFACE (DESCRIBED ABOVE) WILL
      PRODUCE COLOR PLOTS.

      BLACK AND WHITE PLOTS
      ==================================================================
      WHEN PRODUCING BLACK AND WHITE HARDCOPY ON A MAINFRAME THE USER
      SHOULD ADD A DUMMY SUBROUTINE PEN TO THE END OF THE PROGRAM TO
      IGNORE ATTEMPTS TO CHANGE COLOR. ADD THE FOLLOWING SUBROUTINE,

      SUBROUTINE PEN(IPEN)
      RETURN
      END

      CHARACTER SET
      ==================================================================
```

THIS PROGRAM USES COMPUTER AND PLOTTER DEVICE INDEPENDENT SOFTWARE CHARACTERS. THIS PROGRAM COMES WITH A FILE THAT DEFINES THE PEN STROKES REQUIRED TO DRAW ALL CHARACTERS ON AN IBM KEYBOARD (UPPER AND LOWER CASE CHARACTERS, NUMBERS, ETC.) PLUS AN ALTERNATE SET OF ALL UPPER AND LOWER CASE GREEK CHARACTERS AND ADDITIONAL SPECIAL SYMBOLS.

THE SOFTWARE CHARACTER TABLE CONTAINS X AND Y AND PEN POSITIONS TO DRAW EACH CHARACTER. IF YOU WISH TO DRAW ANY ADDITIONAL CHARACTERS OR TO MODIFY THE FONT OF THE EXISTING CHARACTERS YOU NEED ONLY MODIFY THIS TABLE.

CONTROL CHARACTERS

IN THE SOFTWARE CHARACTER TABLE ALL CHARACTERS TO BE PLOTTED WILL HAVE PEN POSITION = 2 (DRAW) OR = 3 (MOVE). IN ADDITION THE TABLE CURRENTLY CONTAINS 4 CONTROL CHARACTERS,

PEN POSITION = 0

SHIFT THE NEXT PRINTED CHARACTER BY X AND Y. 3 CONTROL CHARACTERS ARE PRESENTLY INCLUDED IN THE SOFTWARE CHARACTER TABLE TO ALLOW SHIFTING.

```
{   = SHIFT UP (FOR SUPERSCRIPTS..............X= 0.0, Y= 0.5)
}   = SHIFT DOWN (FOR SUBSCRIPTS..............X= 0.0, Y=-0.5)
\   = SHIFT LEFT 1 CHARACTER (FOR BACKSPACE...X=-1.0, Y= 0.0)
```

PEN POSITION =-1

SELECT THE NEXT PRINTED CHARACTER FROM THE ALTERNATE CHARACTER SET. AT PRESENT THIS CONTROL CHARACTER IS,

```
|   = SWITCH TO ALTERNATE CHARACTER SET
```

THESE 4 CONTROL CHARACTERS ARE ONLY DEFINED BY THE VALUE OF THE PEN POSITION IN THE SOFTWARE CHARACTER TABLE (I.E., THEY ARE NOT HARD WIRED INTO THIS PROGRAM). AS SUCH BY MODIFYING THE SOFTWARE CHARACTER TABLE THE USER HAS THE OPTION OF DEFINING ANY CONTROL CHARACTERS TO MEET SPECIFIC NEEDS.

THESE CHARACTERS MAY BE USED IN CHARACTER STRINGS TO PRODUCE SPECIAL EFFECTS. FOR EXAMPLE, TO PLOT SUBSCRIPT 5, B, SUPERSCRIPT 10 USE THE STRING,

```
}5B{1{0
```

TO PLOT B, SUBSCRIPT 5 AND SUPERSCRIPT 10 WITH THE 5 DIRECTLY BELOW THE 1 OF THE 10 USE THE STRING,

```
B}5\{1{0
```

TO PLOT UPPER CASE GREEK GAMMA FOLLOWED BY THE WORDS TOTAL WIDTH USE THE STRING,

```
|G TOTAL WIDTH
```

NOTE, WHEN THESE CONTROL CHARACTERS ARE USED THEY ONLY EFFECT THE NEXT 1 PRINTED CHARACTER (SEE, ABOVE EXAMPLE OF PLOTTING SUPER-SCRIPT 10 WHERE THE SHIFT UP CONTROL CHARACTER WAS USED BEFORE THE 1 AND THEN AGAIN BEFORE THE 0).

IF THESE 4 CONTROL CHARACTERS ARE NOT AVAILABLE ON YOUR COMPUTER YOU CAN MODIFY THE SOFTWARE CHARACTER TABLE TO USE ANY OTHER 4 CHARACTERS THAT YOU DO NOT NORMALLY USE IN CHARACTER STRINGS (FOR DETAILS SEE THE SOFTWARE CHARACTER TABLE).

STANDARD/ALTERNATE CHARACTER SETS

THE SOFTWARE CHARACTER TABLE CONTAINS 2 SETS OF CHARACTERS WHICH ARE A STANDARD SET (ALL CHARACTERS ON AN IBM KEYBOARD) AND AN ALTERNATE SET (UPPER AND LOWER CASE GREEK CHARACTERS AND SPECIAL CHARACTERS). TO DRAW A CHARACTER FROM THE ALTERNATE CHARACTER SET PUT A VERTICAL STROKE CHARACTER (|) BEFORE A CHARACTER (SEE THE ABOVE EXAMPLE AND THE SOFTWARE CHARACTER TABLE FOR DETAILS). THIS CONTROL CHARACTER WILL ONLY EFFECT THE NEXT 1 PLOTTED CHARACTER.

SUB AND SUPER SCRIPTS

TO DRAW SUBSCRIPT PRECEED A CHARACTER BY }. TO DRAW SUPERSCRIPT PRECEED A CHARACTER BY { (SEE THE ABOVE EXAMPLE AND THE SOFTWARE CHARACTER TABLE FOR DETAILS). THESE CONTROL CHARACTER WILL ONLY EFFECT THE NEXT 1 PLOTTED CHARACTER.

BACKSPACING

TO BACKSPACE ONE CHARACTER PRECEED A CHARACTER BY \ (SEE, THE ABOVE EXAMPLE AND THE SOFTWARE CHARACTER TABLE FOR DETAILS). THIS CONTROL CHARACTER WILL PERFORM A TRUE BACKSPACE AND WILL EFFECT ALL FOLLOWING CHARACTERS IN THE SAME CHARACTER STRING.

SOFTWARE SYMBOL AND LINE TYPE TABLE

THIS PROGRAM ALLOWS UP TO 30 SETS OF DISCRETE POINTS AND/OR 30 CURVES TO APPEAR ON EACH PLOT. EACH SET OF DISCRETE POINTS IS IDENTIFIED BY A SYMBOL (E.G.,A SQUARE OR A TRIANGLE) AND EACH CURVE IS IDENTIFIED BY A LINE TYPE (E.G., A SOLID LINE OR A DASHED LINE). THE 30 SYMBOLS FOR THE SETS OF DISCRETE POINTS AND THE 30 LINE TYPES ARE EACH DESCRIBED BY A SERIES OF X AND Y POSITIONS AND PEN POSITIONS (SIMILAR TO THE SOFTWARE CHARACTER TABLE).

IF YOU WOULD LIKE TO CHANGE THE ORDER IN WHICH SYMBOLS OR LINE TYPES ARE USED MERELY CHANGE THE ORDER OF THE SYMBOLS OR LINE TYPES IN THE TABLE. IF YOU WOULD LIKE TO USE DIFFERENT SYMBOLS OR LINE TYPES YOU CAN MODIFY THE X AND Y AND PEN POSITIONS TO CREATE VIRTUALLY ANY SYMBOL OR LINE TYPE THAT YOU WANT.

THIS PROGRAM IS DISTRIBUTED WITH 2 DIFFERENT SETS OF SOFTWARE SYMBOLS (LINE TYPES ARE THE SAME IN BOTH) AND THE USER IS FREE TO USE EITHER SET. THE STANDARD SET CONTAINS 30 DIFFERENT SYMBOLS AND THE ALTERNATE SET CONTAINS 30 SQUARES WITH A NUMBER OR LETTER CENTERED IN THE SQUARE (FOR DETAILS SEE THE DOCUMENTATION FOR PROGRAM PLOTTAB).

WARNING...THE PROGRAM ASSUMES THAT THE FIRST 30 ENTRIES IN THE SOFTWARE SYMBOL AND LINE TYPE TABLE DESCRIBE 30 SYMBOLS AND THE NEXT 30 ENTRIES DESCRIBE 30 LINE TYPES. YOU CAN RE-ORDER OR REPLACE SYMBOLS OR LINE TYPES, BUT YOU SHOULD NEVER EXCHANGE SYMBOLS AND LINE TYPES AND YOU MUST INSURE THAT AFTER MODIFYING THE TABLE IT STILL CONTAINS 30 SYMBOLS FOLLOWED BY 30 LINE TYPES (SEE, NEXT PARAGRAPH FOR AN EXCEPTION TO THIS RULE).

ALL CURVES SOLID LINES

DATA IN THE ENDF/B OR EXFOR CAN BE EASILY TRANSLATED INTO THE FORMATS READ BY THIS PROGRAM.

OPTIONS
===

IF THE PROGRAM DOES NOT FIND LINE TYPES AFTER THE 30 SYMBOLS IN THE SOFTWARE SYMBOL AND LINE TYPE TABLE IT WILL DRAW ALL CURVES AS SOLID LINES. THEREFORE IF YOU WISH TO DRAW ALL CURVES AS SOLID LINES YOU CAN EITHER MODIFY THE LINE TYPES TO ALL REPRESENT SOLID LINES OR ELSE MERELY DELETE THE LINE TYPES FROM THE END OF THE TABLE.

LINE THICKNESS
===
IF THE INPUT PARAMETERS DO NOT SPECIFY THICK LINES EACH PEN STROKE WILL BE PERFORMED ONLY ONCE. IF THE INPUT PARAMETERS SPECIFIES A LINE THICKNESS (1 TO 10) EACH PEN STROKE WILL BE PERFORMED 1 TO 10 TIMES WITH EACH REPETITION SLIGHTLY OFFSET FROM THE LAST ONE TO CREATE A THICKER LINE. SEE, THE EXAMPLE PLOTS IN THE DOCUMENTATION FOR THIS PROGRAM IN ORDER TO UNDERSTAND THE EFFECT THAT THIS CAN CREATE.

WARNING...SPECIFYING A LINE THICKNESS OF 1 TO 10 CAN CAUSE THIS PROGRAM TO RUN 1 TO 10 TIMES LONGER. THEREFORE LINE THICKNESS SHOULD ONLY BE SPECIFIED FOR FINISHED, HIGH QUALITY PLOTS. THE OFFSET BETWEEN STROKES IS CURRENTLY DEFINED BY THE PROGRAM TO BE 0.002 INCHES. THEREFORE LINE THICKNESS SHOULD ONLY BE SPECIFIED FOR HIGH RESOLUTION PLOTTERS (OTHERWISE YOU WILL BE MERELY WASTING TIME AND YOU WILL NOT BE ABLE TO SEE ANY DIFFERENCES IN THE PLOTS)

WHEN THIS PROGRAM IS RUN ON AN IBM-PC WITH AN ATTACHED HEWLETT-PACKARD 7475A PLOTTER THE PROGRAM WILL AUTOMATICALLY TURN OFF THE THICK LINE OPTION (AVOID WASTING TIME ON THIS LOW RESOLUTION PEN PLOTTER).

***** PLOTTER/GRAPHICS TERMINAL INTERFACE *****************************

IF REQUESTED, THE PROGRAM WILL USE THIS DATA TO DRAW A SET OF

Software characters

This program uses a table of plotter independent characters. The following two pages list all of the characters used by this program. The first page lists the standard characters and the second page the alternate characters (see, comment cards from program for details).

... ALLOWED, X ORDER. FAILURE TO CONFORM TO THIS RULE CAN RESULT IN UNPREDICTABLE RESULTS.

INTERPOLATION OF CURVES

Standard Character Set

	B	N	Z	l	x	<	&
Ø	C	O	a	m	y	%	—
1	D	P	b	n	z	`	!
2	E	Q	c	o	-	¢	¦
3	F	R	d	p	+	;	:
4	G	S	e	q	.	'	"
5	H	T	f	r	=	,	?
6	I	U	g	s	/	~	
7	J	V	h	t	*	@	
8	K	W	i	u	)	#	
9	L	X	j	v	(	$	
A	M	Y	k	w	>	¬	

= 2 - YES..ALL CURVES ONLY ON FIRST PLOT.
(UP TO 30 CURVES)

Alternate Character Set

A	A	N	N	a	α	n	ν	0	∝
B	B	O	O	b	β	o	o	1	∞
C	X	P	Π	c	χ	p	π	2	→
D	Δ	Q	Θ	d	δ	q	θ	3	←
E	E	R	P	e	ε	r	ρ	4	[
F	Φ	S	Σ	f	φ	s	σ	5	]
G	Γ	T	T	g	γ	t	τ	6	≡
H	H	U	Υ	h	η	u	υ	7	≠
I	I	W	Ω	i	ι	w	ω	8	≥
K	K	X	Ξ	k	κ	x	ξ	9	≤
L	Λ	Y	Ψ	l	λ	y	ψ		
M	M	Z	Z	m	μ	z	ζ		

= 1 - LINEAR (SCALED TO
=-1 - LINEAR (SCALED TO LOWER 0.0 LIMIT)
= OTHERWISE DEFAULT OF LOG

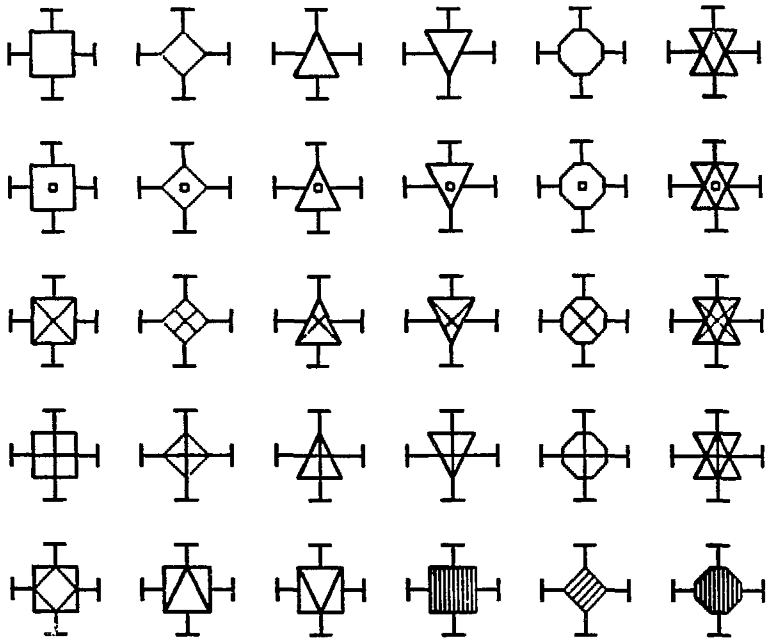
THE ABOVE 3 LINES ARE READ FOR EACH PLOT. PROGRAM EXECUTION

Symbols to identify sets of discrete data points

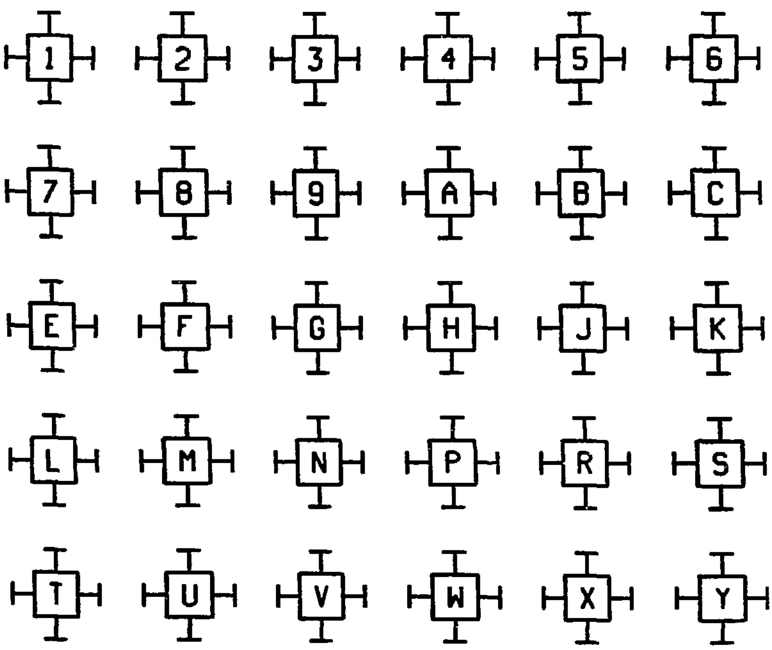
This program is distributed with two sets of software symbols which are used to identify sets of descrete data points. The user is free to use either set of symbols. The following page illustrates the standard and alternate set of symbols.

IN ORDER TO CREATE OTHER COMBINATIONS OF CURVES AND PLOTS IT IS USUALLY EASIER TO EDIT YOUR CURVE AND POINT FILES TO CONTAIN THE THE DATA TO AP[illegible]N THE PLOTS THAN TO INCLUDE MORE INPUT OPTIONS

Standard Symbols



Alternate Symbols



EXAMPLE NO. 3 UNIT 4 INPUT

TO COMPARE THE ENDF/B-IV 27-CO-59 (N,2N) EVALUATION TO ALL

Example JCL deck

(NOTE, BLANK CARD TERMINATES CURVE).

ENDL84 27-CO-59 (N,2N)

1.12000+ 7 0.00000+ 0

```
//RNC1 JOB (NO,P),P-14-CULLEN,CLASS=I,MSGCLASS=X,NOTIFY=RNC,
//  TIME=(0,10)
//*
//*     PLOT CURVE AND/OR DISCRETE POINTS FROM TABULATED DATA
//*
//*     FOR A DETAILED DESCRIPTION OF ALL INPUT PARAMETERS SEE THE
//*     DOCUMENTATION FOR PROGRAM PLOTTAB.
//*
//JOBLIB  DD  DSN=XNDC.EVALLIB,DISP=SHR
//PASS1  EXEC  PGM=PLOTTAB
//FT06F001  DD  DSN=XNDC.PLOTTAB.REPORT(PLOTTAB),DISP=SHR
//FT10F001  DD  DSN=XNDC.PLOTTAB.SEND(CURVES),DISP=SHR
//FT11F001  DD  DSN=XNDC.PLOTTAB.SEND(POINTS),DISP=SHR
//FT12F001  DD  DSN=XNDC.PLOTTAB.SEND(CHARACTR),DISP=SHR
//FT14F001  DD  DSN=XNDC.PLOTTAB.SEND(SYMBOLS1),DISP=SHR
//GRAFWARE  DD  SYSOUT=P,DEST=CENTRAL
//PLOTTAPE  DD  SYSOUT=P
//FT04F001  DD  *
          3          3          0          0          0          1
Incident Electron Energy                                 eV
Cross Section                                            cm{2
Electron Impact Ionization                         Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-
 9.00000+ 1 1.00000+ 4          1          1          0          1
Electron Impact Ionization                         Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-  (Threshold behaviour)
 1.30000+ 2 2.50000+ 2          1          1          1          1
Electron Impact Ionization                         Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-  (Autoionization resonance behaviour)
 2.00000+ 2 1.00000+ 3          1          1          1          1
Electron Impact Ionization                         Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-  (Resonance recombination)
 4.00000+ 2 8.00000+ 2          1          1          1          1
```

```
L.R.VEESER, ET AL. (77)                        27-CO-59 (N,2N)
 1.10000+ 7 1.10000+ 6 1.10000+ 6 1.10000- 4 2.30000- 4 1.10000- 4
 1.20000+ 7                       1.20000- 3
```

Example output listing

DETAIL AS POSSIBLE, IDENTIFY THE VERSION OF THE PROGRAM THAT YOU

```
PLOT TABULATED DATA (PLOTTAB VERSION 87-2)
======================================================================
PLOT CONTINUOUS CURVE.............YES  (TOGETHER - ON ALL PLOTS)
PLOT DISCRETE POINTS..............YES  (TOGETHER - ON ALL PLOTS)
PLOT SIZE.........................FULL
TYPE OF GRID......................TICK MARKS
SHOULD RATIOS BE PLOTTED..........NO
LINE THICKNESS....................   1
======================================================================
X AXIS LABEL AND UNITS............ Incident Electron Energy (eV)
Y AXIS LABEL AND UNITS............ Cross Section (cm{2)
======================================================================
======================================================================
PLOT TITLE
......................................................................
Electron Impact Ionization                          Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-
======================================================================
REQUESTED X RANGE.................  9.0000E+01   1.0000E+04
PLOT X ERROR BARS.................YES
PLOT Y ERROR BARS.................YES
X PLANE ON PLOTS (IF POSSIBLE)....LOG
Y PLANE ON PLOTS (IF POSSIBLE)....LINEAR
======================================================================
X LIMITS (PLANE)..................  9.0000E+01  1.0000E+04 (LOG)
Y LIMITS (PLANE).................. -5.5500E-21  1.1000E-18 (LINEAR)
======================================================================
CONTINUOUS CURVES
......................................................................
INDEX DESCRIPTION                  POINTS
......................................................................
    1 Recommended                      92
    2 Lotz (1967)                      83
    3 Burgess et al (1983)             87
======================================================================
DISCRETE POINTS
......................................................................
INDEX DESCRIPTION                  POINTS
......................................................................
    1 Donets et al (1977)               8
    2 Crandall et al (1979)            14
    3 Crandall et al (1986)            25
    4 Jakubowitz (1980) (CBE)          19
======================================================================
PLOT TITLE
......................................................................
Electron Impact Ionization                          Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-  (Threshold behaviour)
======================================================================
REQUESTED X RANGE.................  1.3000E+02   2.5000E+02
PLOT X ERROR BARS.................YES
PLOT Y ERROR BARS.................YES
X PLANE ON PLOTS (IF POSSIBLE)....LINEAR
Y PLANE ON PLOTS (IF POSSIBLE)....LINEAR
======================================================================
X LIMITS (PLANE)..................  1.3000E+02  2.5000E+02 (LINEAR)
Y LIMITS (PLANE).................. -5.5500E-21  8.2001E-19 (LINEAR)
======================================================================
CONTINUOUS CURVES
......................................................................
INDEX DESCRIPTION                  POINTS
......................................................................
```

CONTINUOUS STRING IT IS NOT RECOMMENDED THAT YOU USE THIS PROGRAM.

* THIS PROGRAM USING THE FORTRAN-77 CONVENTION FOR TESTING FOR READING ERRORS AND END OF FILE DURING READS, E.G.,

```
   1 Recommended                    34
   2 Lotz (1967)                    34
   3 Burgess et al (1983)           38
=================================================================
DISCRETE POINTS
.................................................................
INDEX DESCRIPTION                  POINTS
.................................................................
   1 Crandall et al (1979)          3
   2 Crandall et al (1986)          8
   3 Jakubowitz (1980) (CBE)        5
=================================================================
PLOT TITLE
.................................................................
Electron Impact Ionization                        Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-  (Autoionization resonance behaviour)
=================================================================
REQUESTED X RANGE.................  2.0000E+02   1.0000E+03
PLOT X ERROR BARS.................YES
PLOT Y ERROR BARS.................YES
X PLANE ON PLOTS (IF POSSIBLE)....LINEAR
Y PLANE ON PLOTS (IF POSSIBLE)....LINEAR
=================================================================
X LIMITS (PLANE)..................  2.0000E+02  1.0000E+03 (LINEAR)
Y LIMITS (PLANE)..................  3.8001E-19  1.1000E-18 (LINEAR)
=================================================================
CONTINUOUS CURVES
.................................................................
INDEX DESCRIPTION                  POINTS
.................................................................
   1 Recommended                    33
   2 Lotz (1967)                    29
   3 Burgess et al (1983)           29
=================================================================
DISCRETE POINTS
.................................................................
INDEX DESCRIPTION                  POINTS
.................................................................
   1 Crandall et al (1979)          10
   2 Crandall et al (1986)          18
   3 Jakubowitz (1980) (CBE)        16
=================================================================
PLOT TITLE
.................................................................
Electron Impact Ionization                        Cross Section
e{- + O{5{+ |2 e{- + O{6{+ + e{-  (Resonance recombination)
=================================================================
REQUESTED X RANGE.................  4.0000E+02   8.0000E+02
PLOT X ERROR BARS.................YES
PLOT Y ERROR BARS.................YES
X PLANE ON PLOTS (IF POSSIBLE)....LINEAR
Y PLANE ON PLOTS (IF POSSIBLE)....LINEAR
=================================================================
X LIMITS (PLANE)..................  4.0000E+02  8.0000E+02 (LINEAR)
Y LIMITS (PLANE)..................  6.2001E-19  1.0200E-18 (LINEAR)
=================================================================
CONTINUOUS CURVES
.................................................................
INDEX DESCRIPTION                  POINTS
.................................................................
   1 Recommended                    17
   2 Lotz (1967)                    14
```

END

CHARACTER SET

==

3 Burgess et al (1983) 14

==

DISCRETE POINTS

INDEX	DESCRIPTION	POINTS
1	Crandall et al (1979)	7
2	Crandall et al (1986)	9
3	Jakubowitz (1980) (CBE)	10

==

END OF RUN 4 PLOTS GENERATED

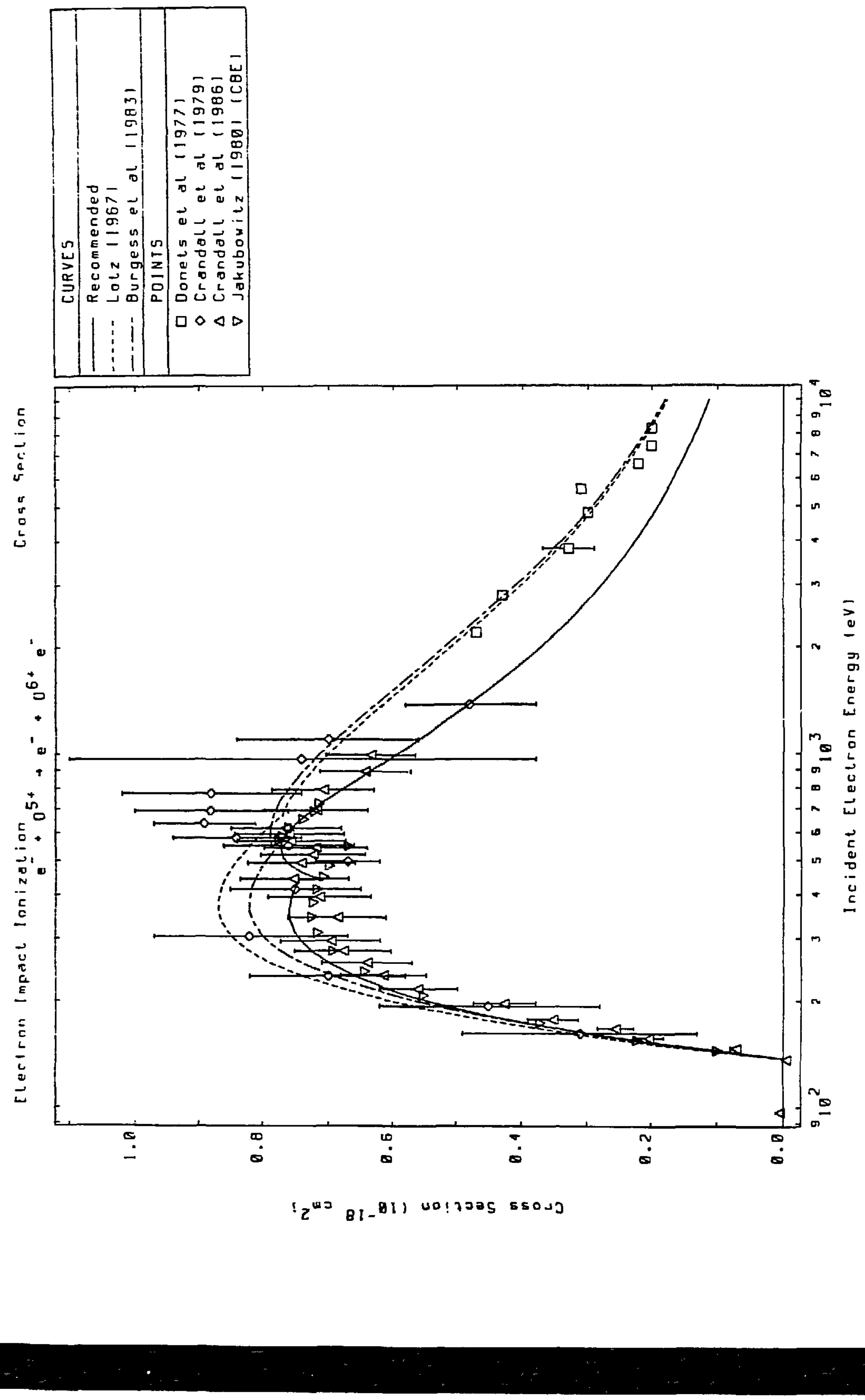
(SEE, ABOVE EXAMPLE OF PLOTTING SUPER-
SCRIPT 10 WHERE THE SHIFT UP CONTROL CHARACTER WAS USED BEFORE THE
1 AND THEN AGAIN BEFORE THE 0).

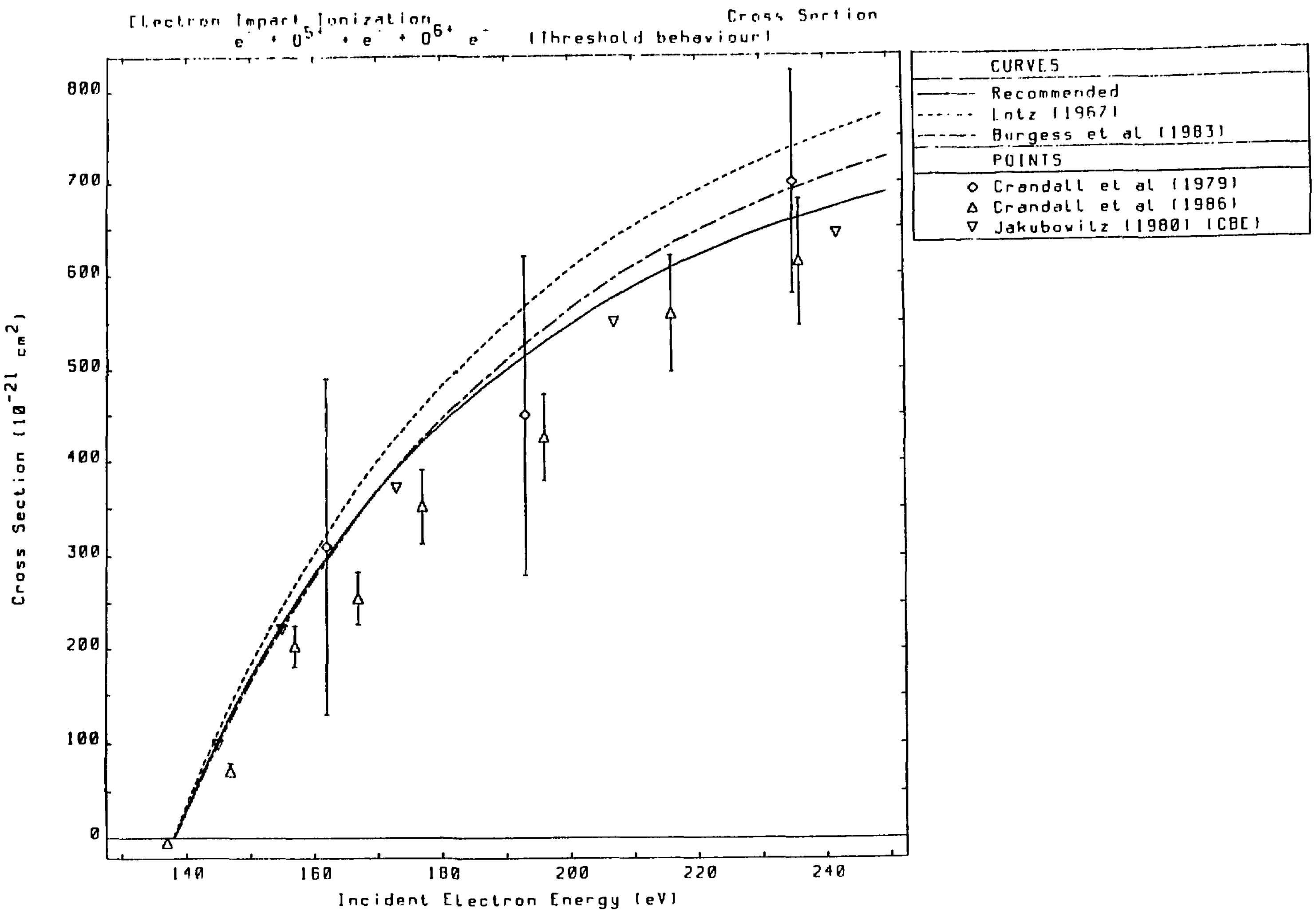
Example Plots

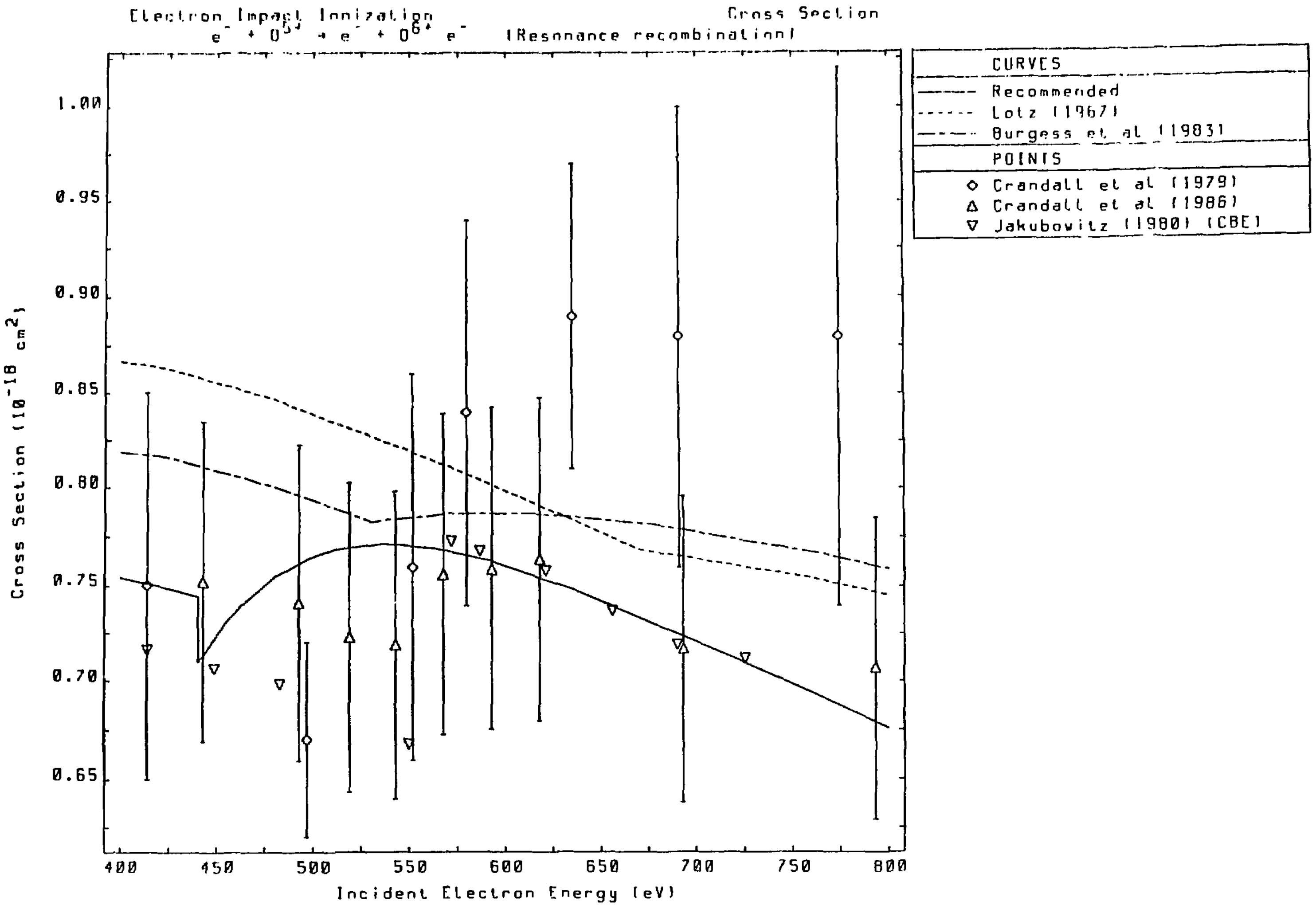
The following 4 pages illustrate the 4 plots which should be obtained when the example problem distributed with this program is run.

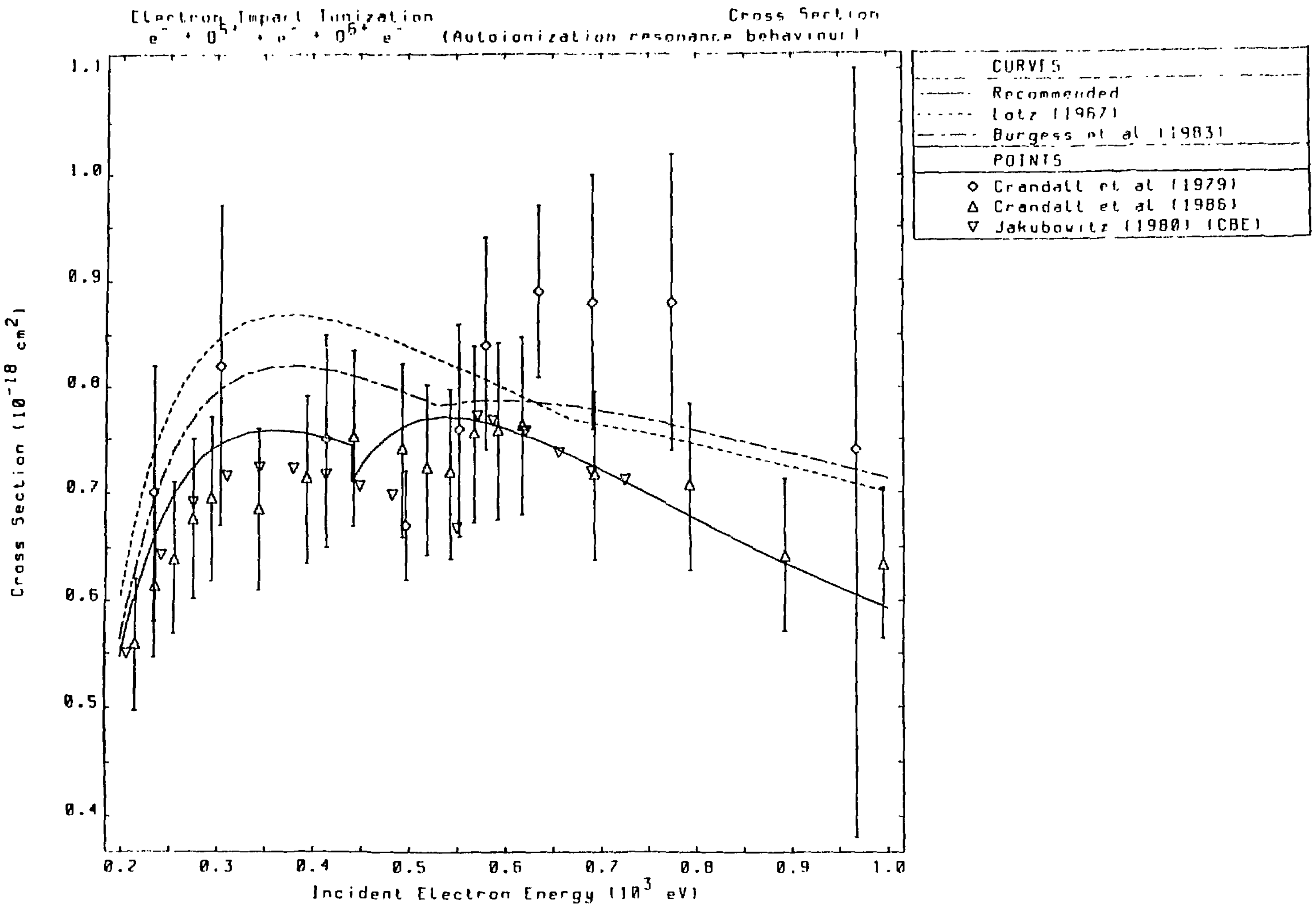
These 4 plots are followed by additional plots which illustrate the effect of using each input option.

ALL CURVES SOLID LINES



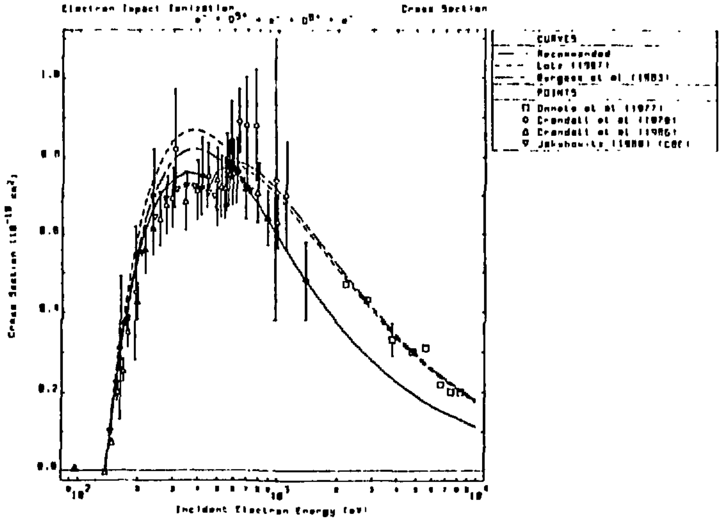

Electron Impact Ionization
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ e⁻
Cross Section
(Threshold behaviour)
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10⁻²¹ cm²)
0
100
200
300
400
500
600
700
800
140
160
180
200
220
240
Incident Electron Energy (eV)


Electron Impact Ionization
$e^- + O^{5+} \rightarrow e^- + O^{6+}\ e^-$ (Resonance recombination)
Cross Section
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10^{-18} cm^2)
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
400
450
500
550
600
650
700
750
800
Incident Electron Energy (eV)

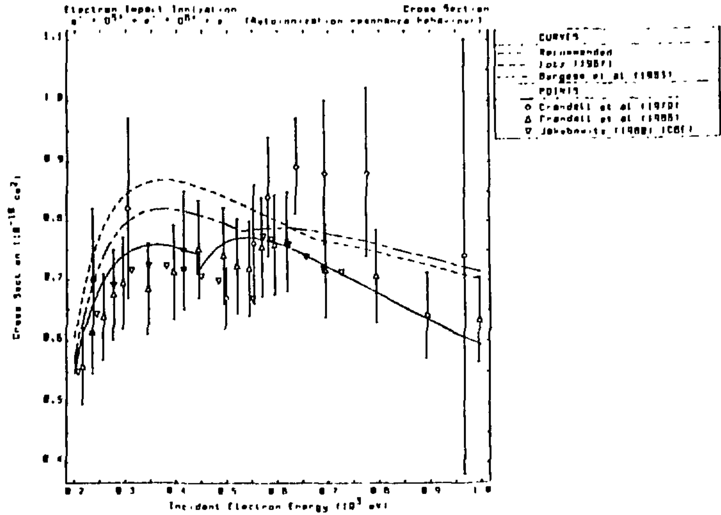

Electron Impact Ionization
Cross Section
(Autoionization resonance behaviour)
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10^-18 cm^2)
Incident Electron Energy (10^3 eV)

Half size plots

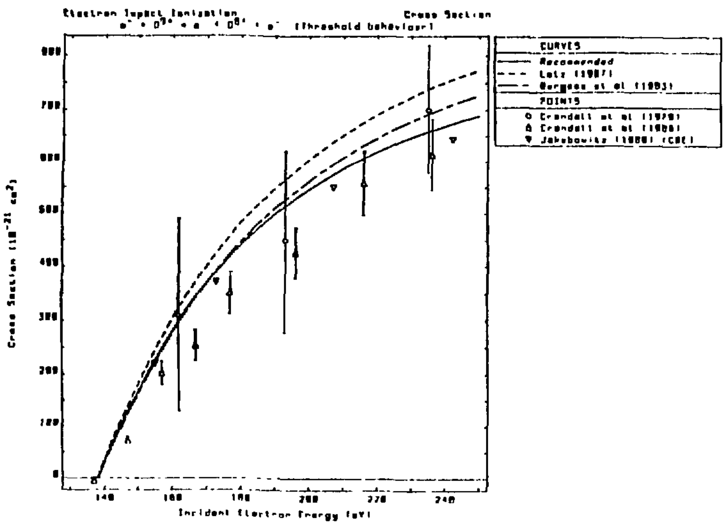
Plot size is controlled by columns 23-33 of the first input line (see, comment cards from program for details). The preceding 4 pages present plots corresponding to the example input distributed with this program. The following page presents the same data in half-size plot mode (i.e., change columns 23-33 from 0 to 1 and use the same example problem).



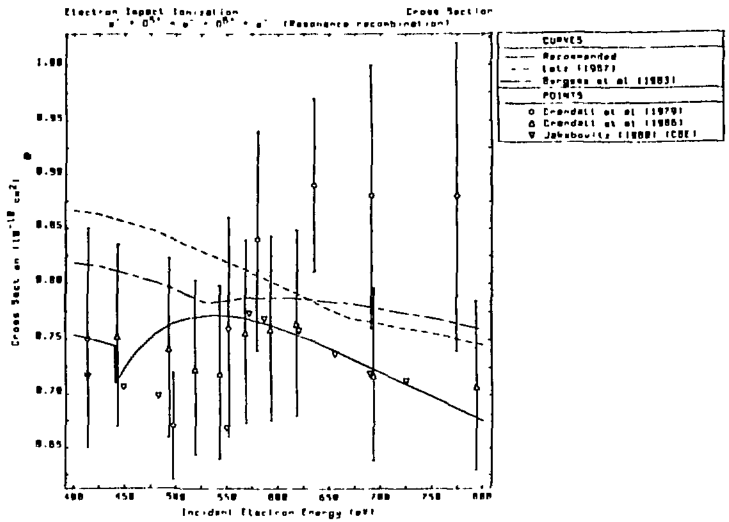
Electron Impact Ionization
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻
Cross Section
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10⁻¹⁸ cm²)
Incident Electron Energy (eV)



Electron Impact Ionization
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻ (Autoionization resonance behavior)
Cross Section
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10⁻¹⁸ cm²)
Incident Electron Energy (10³ eV)



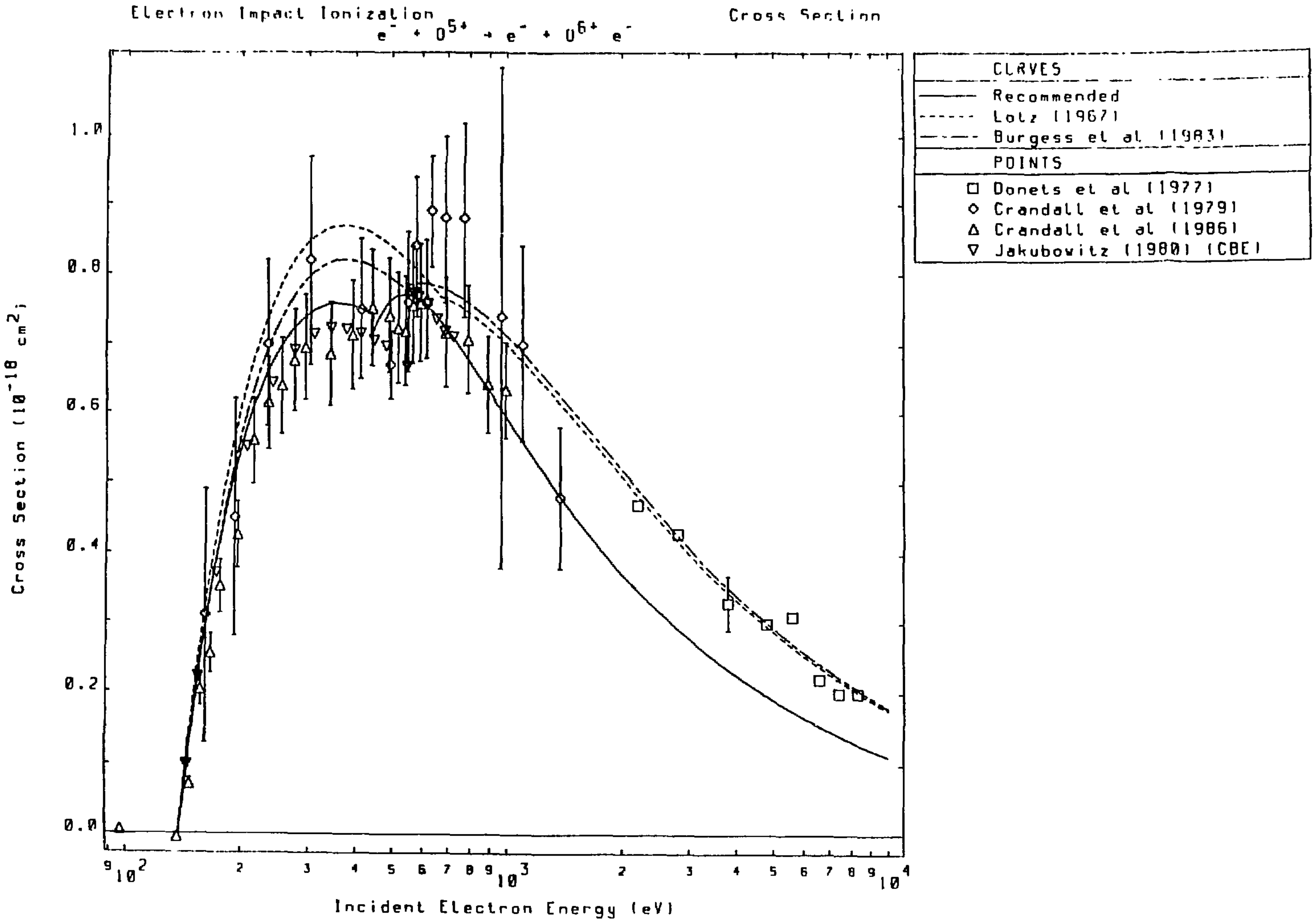
Electron Impact Ionization
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻ (Threshold behavior)
Cross Section
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10⁻²¹ cm²)
Incident Electron Energy (eV)



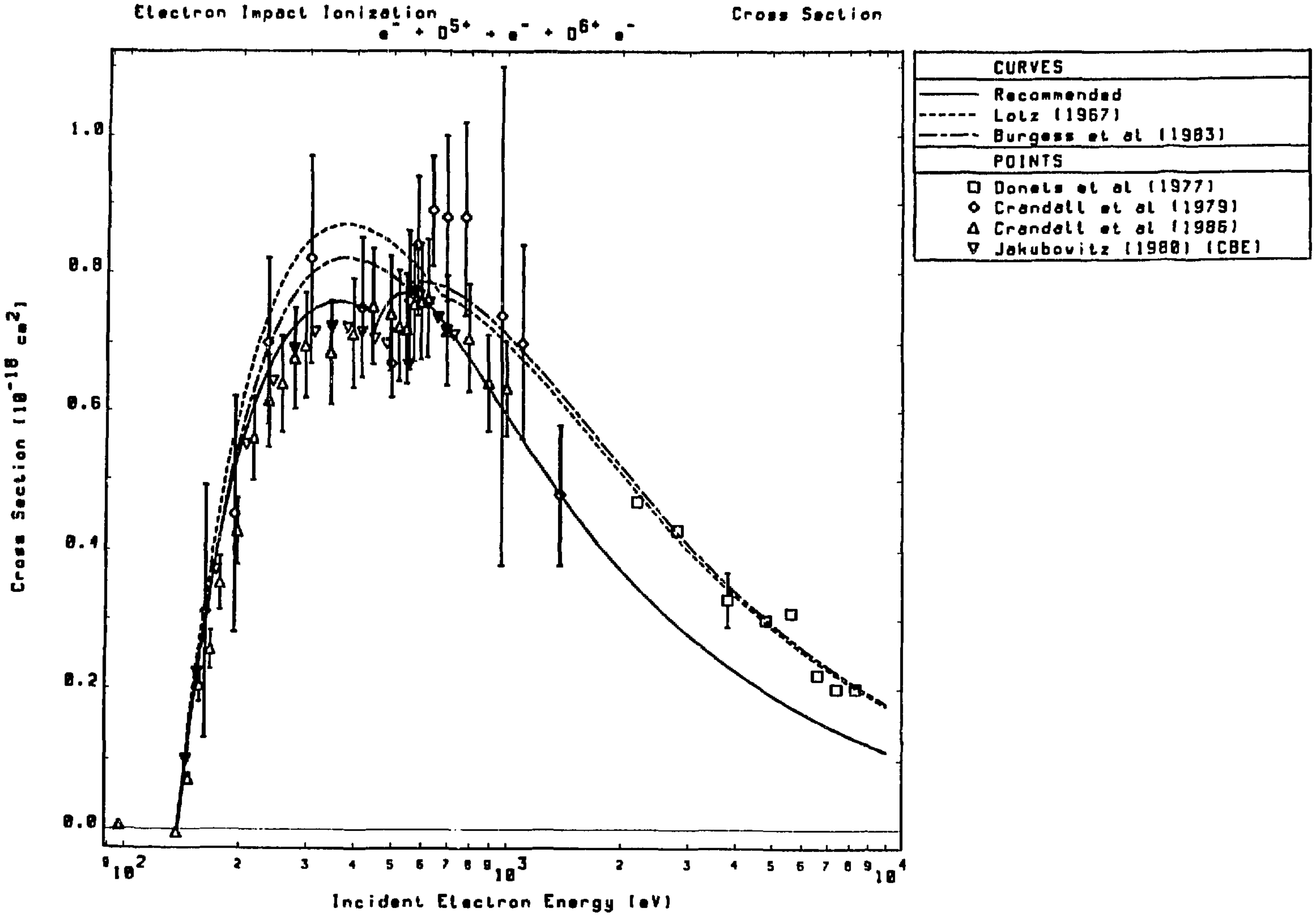
Electron Impact Ionization
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ + e⁻ (Resonance recombination)
Cross Section
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10⁻¹⁸ cm²)
Incident Electron Energy (eV)

Type of grid and line thickness

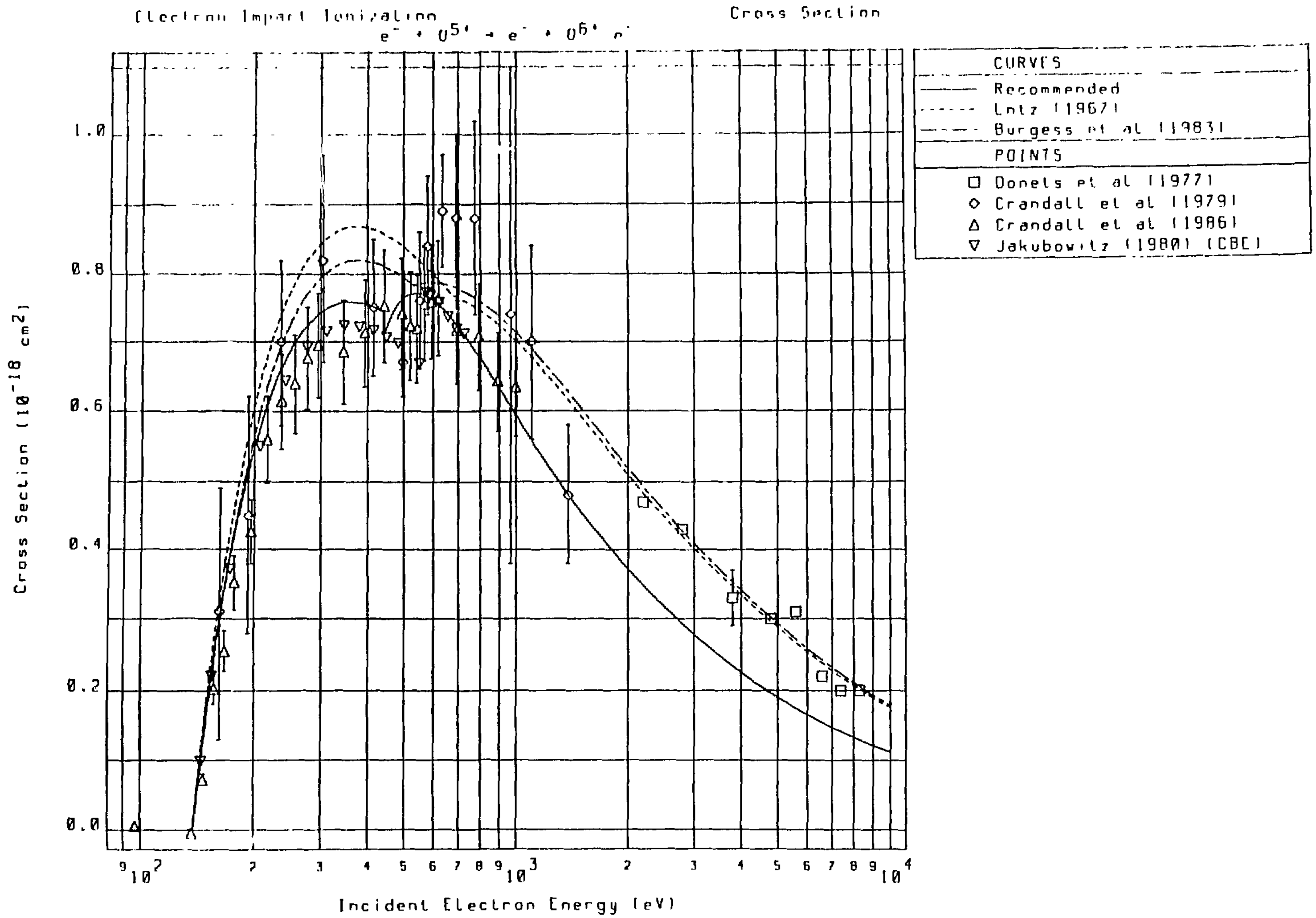
This program can produce plots containing one of three grid types (1) tick marks on border, (2) solid grid lines or (3) dashed grid lines. The program can also produce plots with normal width lines or with thicker lines. When thicker lines are requested all curves, points and characters will be thicker and the only thing which will not be thicker is the grid. With this convention thicker lines are particularly useful to help distinquish data from the grid. The following six pages illustrate the results obtained using each of the three grid types (controlled by columns 34-44 of the first input line) with line thickness 0 and 3 (controlled by columns 56-66 of the first input line).



Electron Impact Ionization
Cross Section
e⁻ + O5+ → e⁻ + O6+ e⁻
Cross Section (10^-18 cm^2)
1.0
0.8
0.6
0.4
0.2
0.0
Incident Electron Energy (eV)
10^2
10^3
10^4
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)



Electron Impact Ionization
Cross Section
$e^- + O^{5+} \rightarrow e^- + O^{6+}\ e^-$
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10^{-18} cm^2)
1.0
0.8
0.6
0.4
0.2
0.0
10^2
10^3
10^4
Incident Electron Energy (eV)



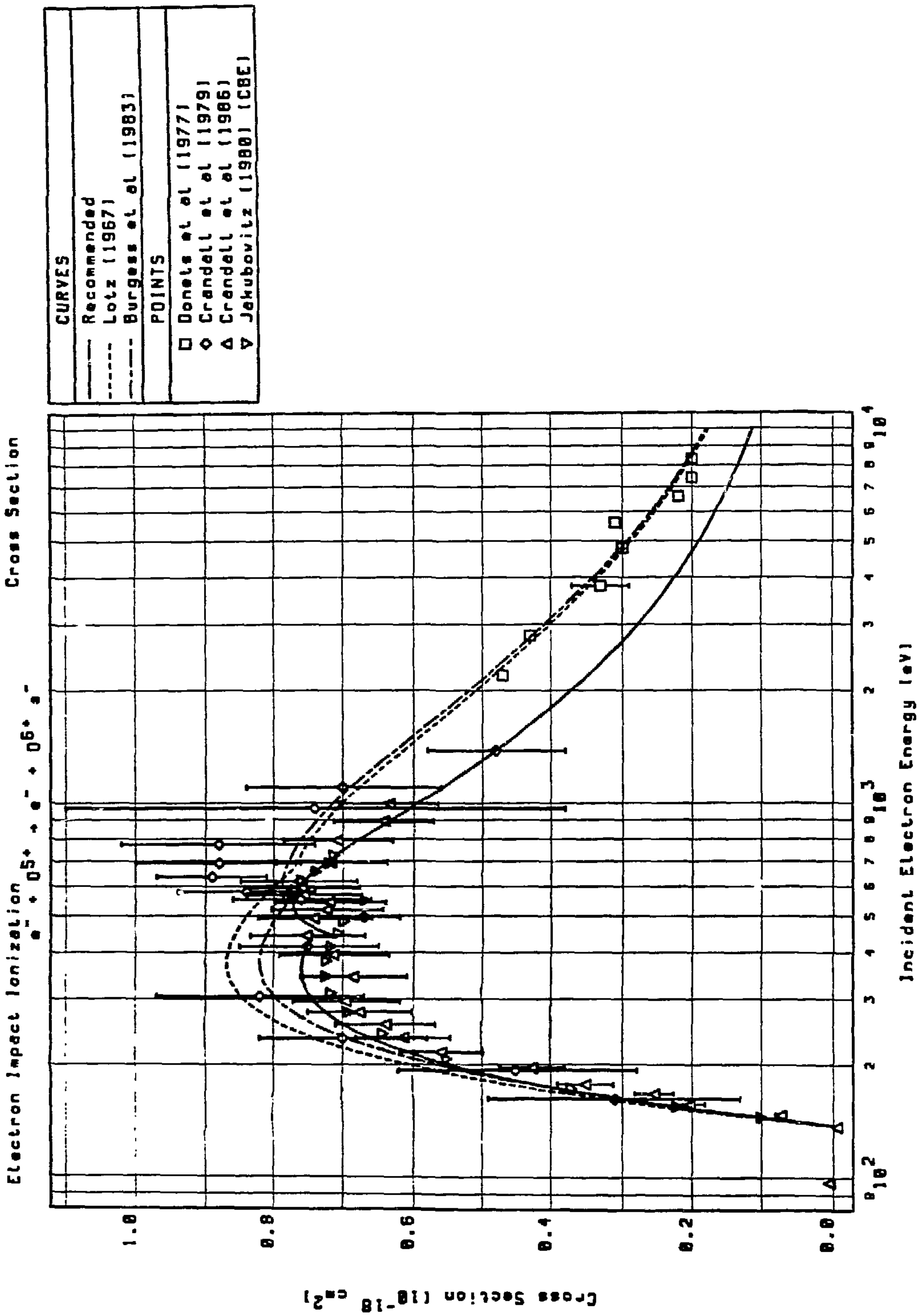
Electron Impact Ionization
$e^- + O^{5+} \rightarrow e^- + O^{6+} e^-$
Cross Section
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10^{-18} cm^2)
1.0
0.8
0.6
0.4
0.2
0.0
9
10^2
2
3
4
5
6
7
8
9
10^3
2
3
4
5
6
7
8
9
10^4
Incident Electron Energy (eV)

CONTINUOUS CURVES

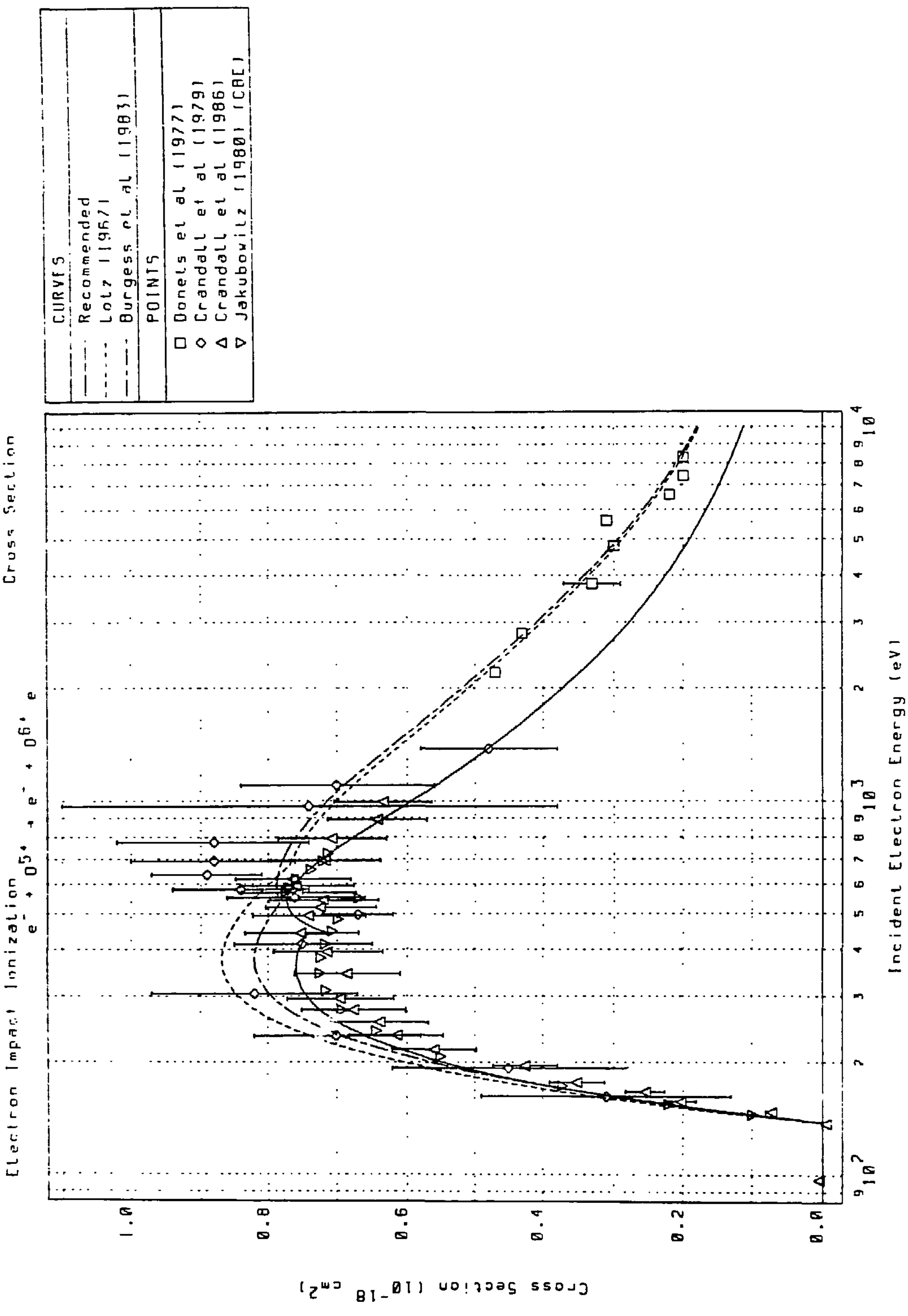
....

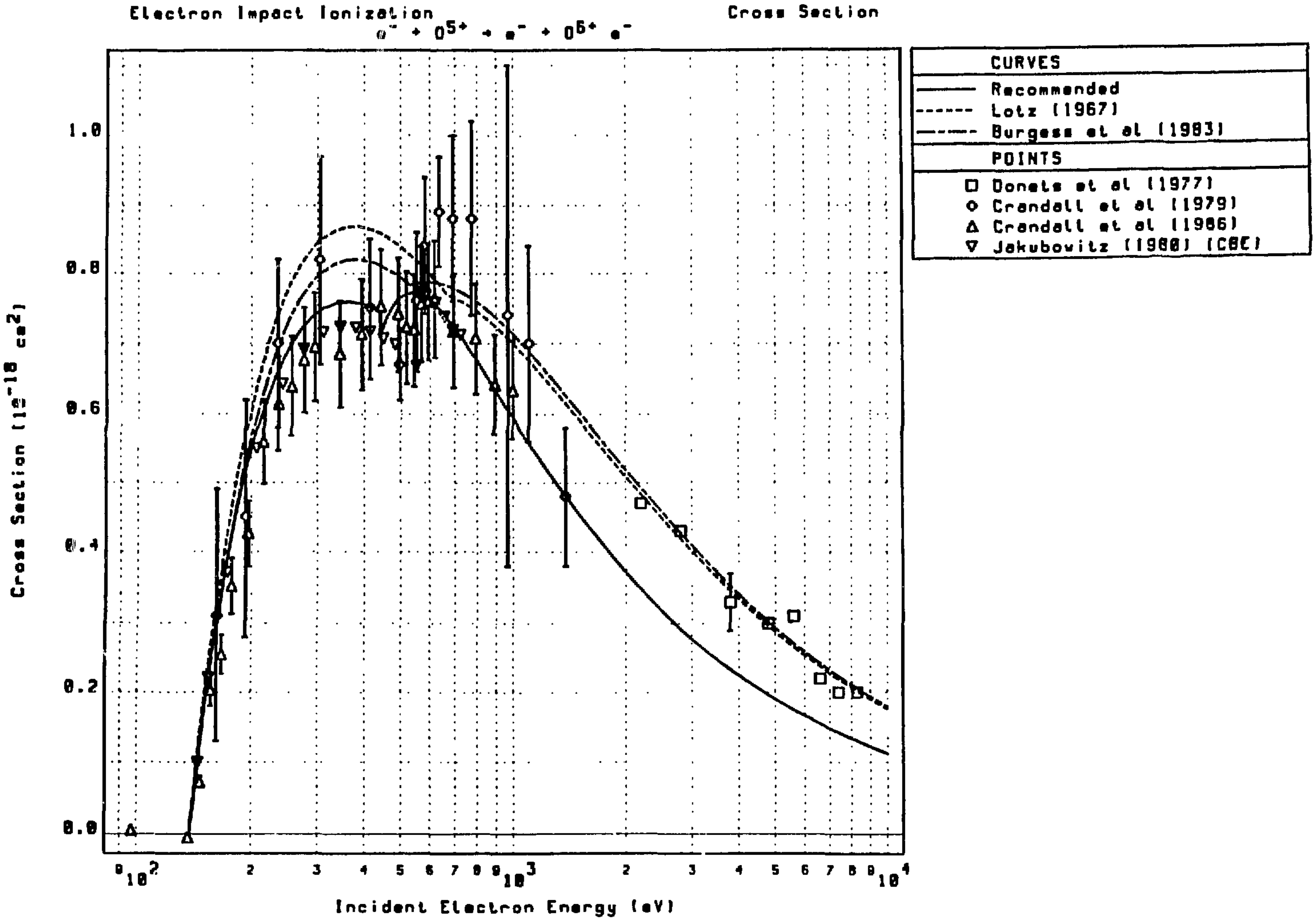
INDEX DESCRIPTION POINTS

....



1	Recommended	17
2	Lotz (1967)	14

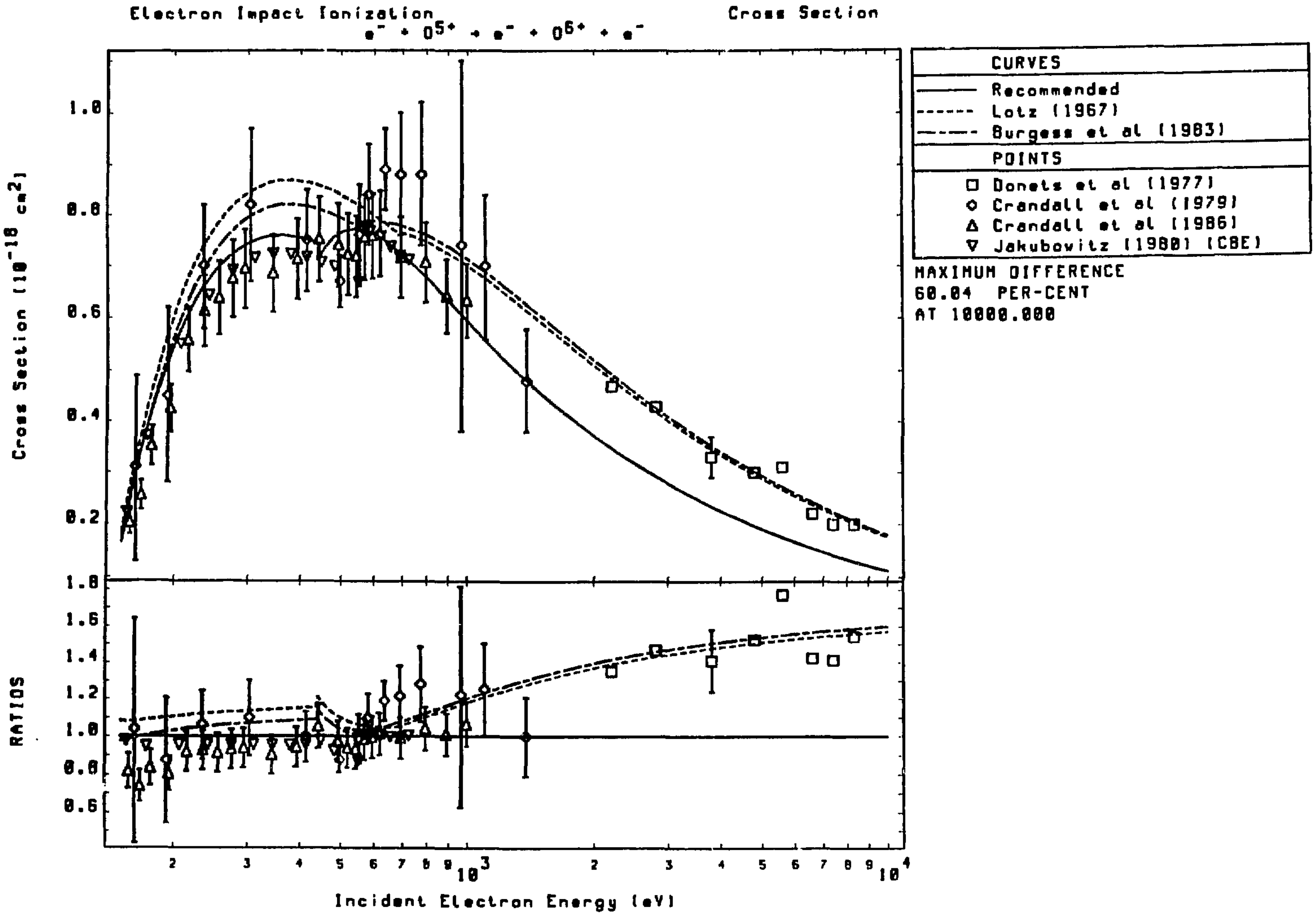




Electron Impact Ionization
Cross Section
e⁻ + O⁵⁺ → e⁻ + O⁶⁺ e⁻
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10⁻¹⁸ cm²)
1.0
0.8
0.6
0.4
0.2
0.0
10²
2
3
4
5
6
7
8
9
10³
10⁴
Incident Electron Energy (eV)

Ratios

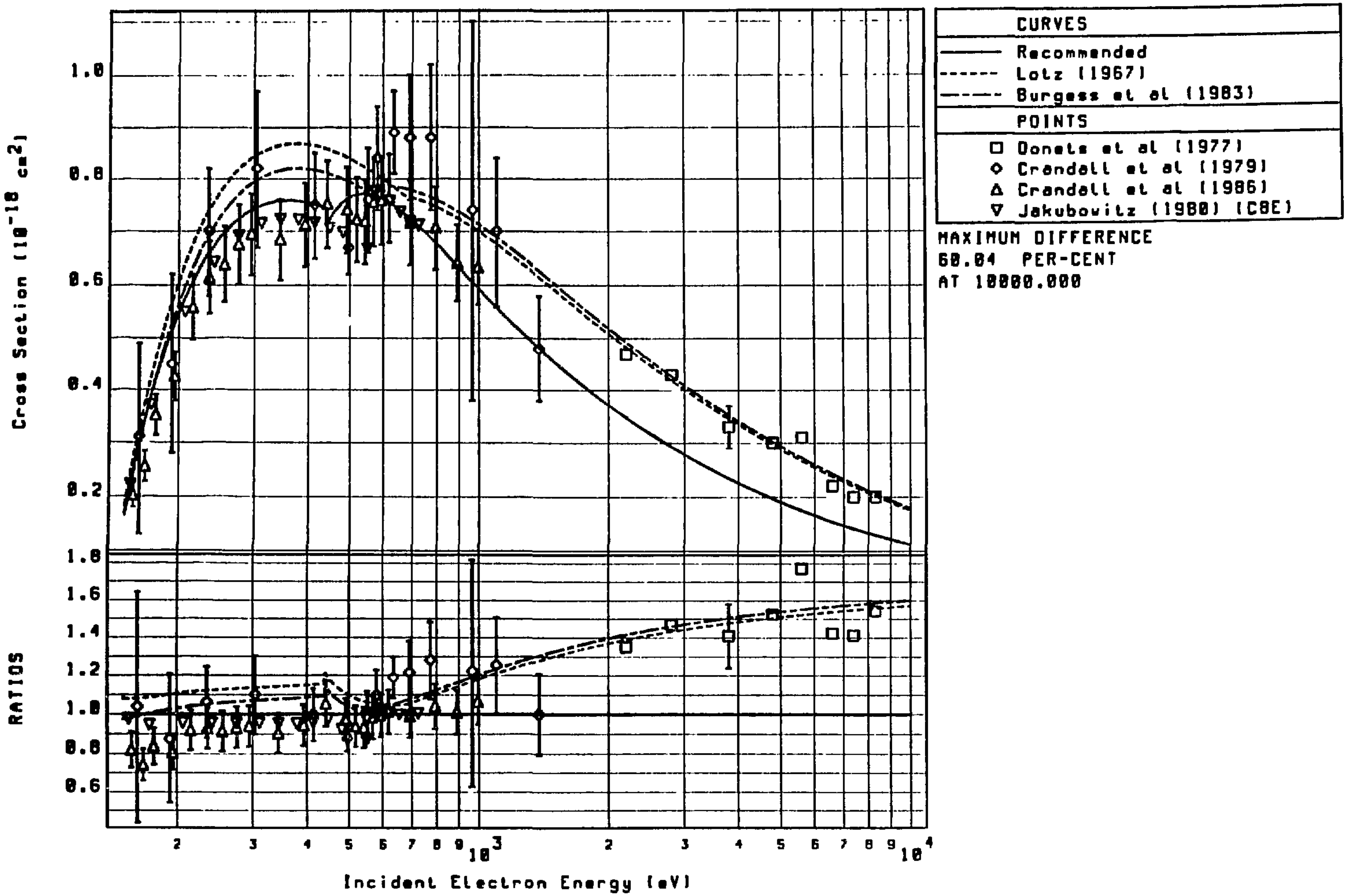
When comparing the results obtained using different models and/or experimental data this program can be used to quantitatively define differences and to indicate the position (x value) and magnitude of the largest difference. This is done by plotting not only all data, but also the ratio of all data to the first curve. The following three pages illustrate the results obtained by specifying that ratios should be plotted (controlled by columns 45-55 of the first input line); results are presented using line thickness 3 and each of the three available grid types.



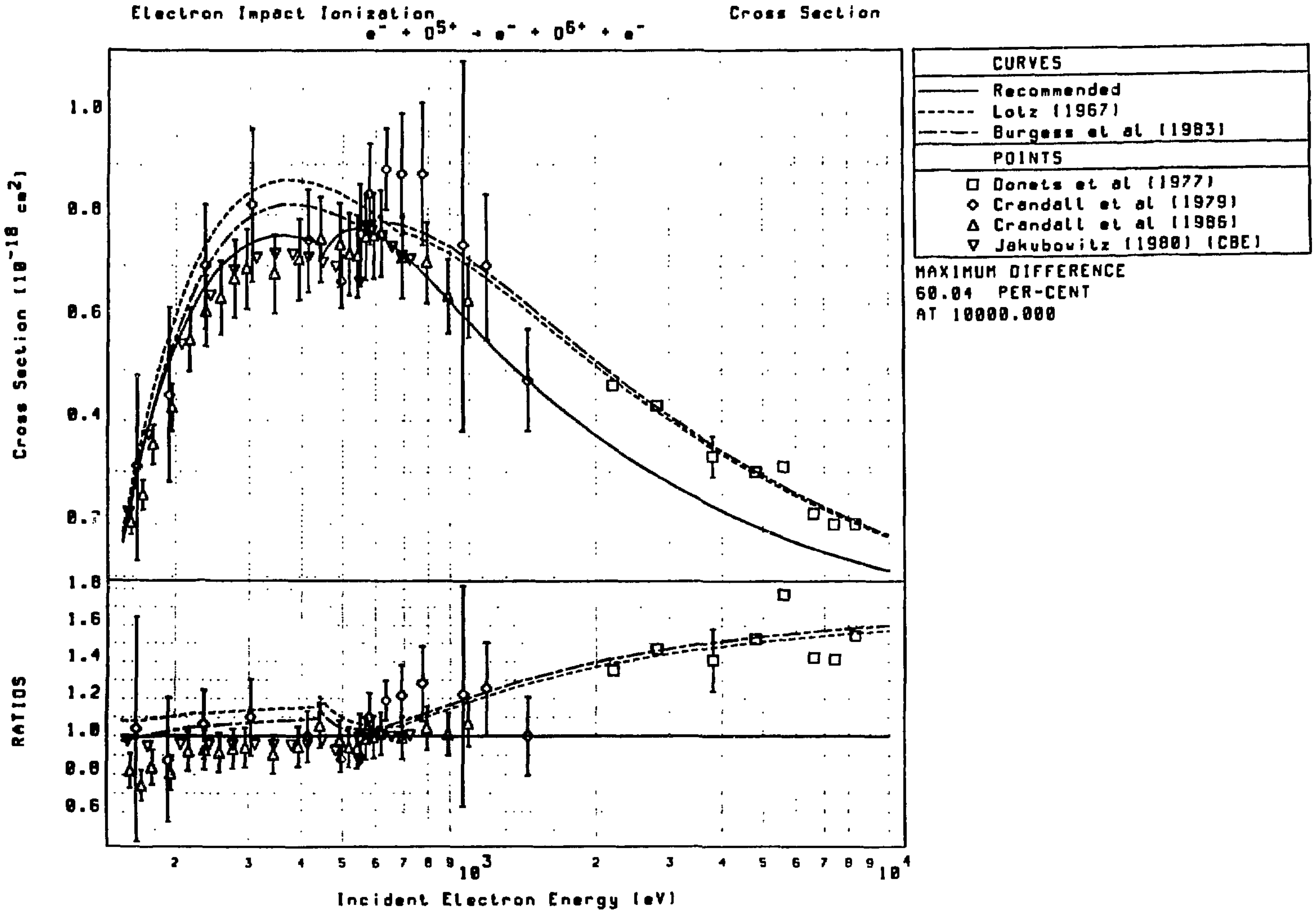
Electron Impact Ionization
Cross Section
e⁻ + O5+ → e⁻ + O6+ + e⁻
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
MAXIMUM DIFFERENCE
60.04 PER-CENT
AT 10000.000
Cross Section (10^-18 cm^2)
RATIOS
Incident Electron Energy (eV)

Electron Impact Ionization Cross Section

$e^- + O^{5+} \rightarrow e^- + O^{6+} + e^-$



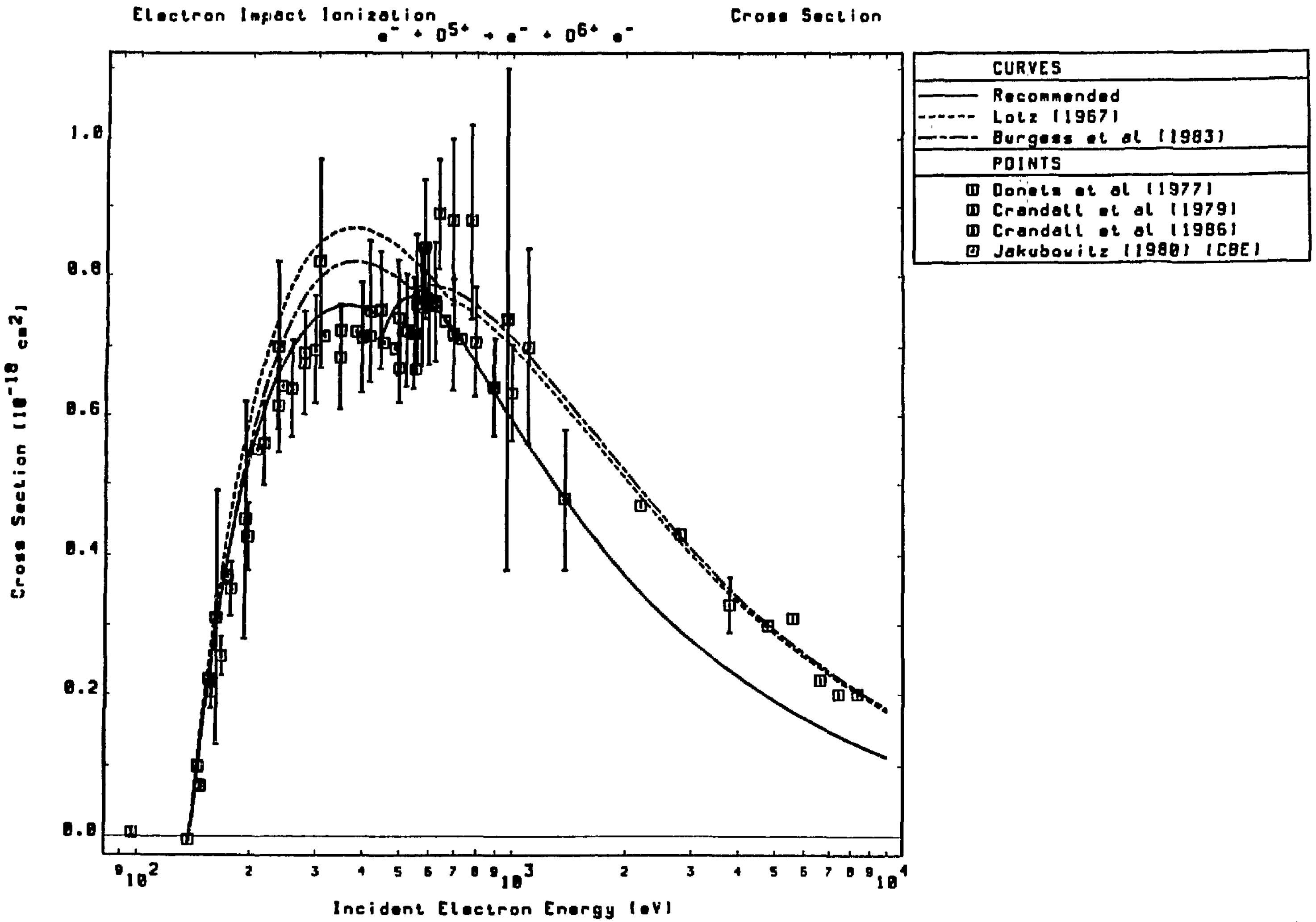
MAXIMUM DIFFERENCE
60.04 PER-CENT
AT 10000.000



Electron Impact Ionization
Cross Section
e⁻ + O5+ → e⁻ + O6+ + e⁻
Cross Section (10^-18 cm^2)
RATIOS
Incident Electron Energy (eV)
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
MAXIMUM DIFFERENCE
60.04 PER-CENT
AT 10000.000

Alternate symbols

All of the preceding plots present results obtained using the standard symbol set to identify sets of discrete points (square, diamond, triangle, etc.). The following plot presents results obtaining using the alternate symbol set (a square with a character centered in the square). The standard and alternate symbol sets are both distributed with the program as two data files. The user can control which set of symbols is used by specifying either the standard or alternate symbol set as File 14 during execution (see, example JCL deck).


Electron Impact Ionization
Cross Section
e⁻ + O5+ → e⁻ + O6+ e⁻
CURVES
Recommended
Lotz (1967)
Burgess et al (1983)
POINTS
Donets et al (1977)
Crandall et al (1979)
Crandall et al (1986)
Jakubowitz (1980) (CBE)
Cross Section (10-18 cm2)
Incident Electron Energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
9
10^2
2
3
4
5
6
7
8
9
10^3
2
3
4
5
6
7
8
9
10^4